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# NATIONAL BUREAU OF STANDARDS REPORT

8906

## FOURTH PRELIMINARY REPORT ON A SURVEY OF

### THERMODYNAMIC PROPERTIES OF THE COMPOUNDS OF THE ELEMENTS CHNOPS

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Progress Report for the Period 1 February to 30 June 1965

to

National Aeronautics and Space Administration

1 July 1965



U.S. DEPARTMENT OF COMMERCE  
NATIONAL BUREAU OF STANDARDS

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**NBS REPORT**

8906

## A SURVEY OF THERMODYNAMIC PROPERTIES OF THE COMPOUNDS OF THE ELEMENTS CHNOPS

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Heat Division, Institute for Basic Standards

Progress Report for the Period 1 February to 30 June 1965

to

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

Contract No. R-138

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**U. S. DEPARTMENT OF COMMERCE  
NATIONAL BUREAU OF STANDARDS**

## FOREWORD

A study at the National Bureau of Standards (NBS), of which this is the fourth progress report, has been undertaken to meet the need of the National Aeronautics and Space Administration (NASA) for thermodynamic information on biologically related materials important to the space program for several reasons. Among these reasons are the necessity of inferring the maximum amount of useful chemistry of incompletely accessible environments, for which only limited information is available, the possibility of the occurrence of organic compounds naturally synthesized under primitive conditions, and the possibility of theoretically recovering part of the prebiological history of the earth.

This program is being carried out under the technical supervision of Dr. George Jacobs of NASA, and with the consultation of Dr. Harold Morowitz of the Yale University, Department of Molecular Biology and Biophysics, and Dr. C. W. Beckett of the Heat Division, IBS (NBS). The contract (Contract No. R-138) was initiated 1 May 1964 and extended 29 April 1965. This report covers the fourth quarter and the supplementary two months of the term of the contract.

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\_\_\_\_\_  
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# TABLE OF CONTENTS

	<u>Page</u>
Foreword . . . . .	i
Introduction . . . . .	1
Section I. Survey of Heat Capacity, Enthalpy, and Entropy Data on CHNOPS Compounds . . .	3
Bibliography . . . . .	41
Section II. Heats and Free Energies of Formation of Compounds of C, H, N, O, P, and S . .	69
Table 1. Selected Heats of Combustion and Heats of Formation of Certain Organic Compounds . . . . .	71
Table 2. Free Energies of Formation of Certain Amino Acids . . . . .	74
Table 3. Supplementary List of Compounds of CHNOPS Containing Not More Than One C Atom per Molecule . . . . .	76
Summary Index to Tables contained in NBS Reports 8521, 8595, 8641, and 8906 . .	86

## INTRODUCTION

Since this report contains several references to material from earlier reports, it seems appropriate to summarize briefly the material given in the three previous progress reports. A summary index at the end of this report provides a list of tables appearing in all the progress reports of the contract, including the present one, and can serve as a guide to the information provided in the study. Some comments on the tables and the relationships between them are given below.

The first quarterly report (NBS Report 8521) contains two preliminary compilations of data published on biologically-related substances. One is a tabulation of temperature ranges over which heat capacity and relative enthalpy measurements have been made, entropies, and references, for a wide variety of organic compounds (pp. 5-32). The other is a preliminary bibliography of sources containing data relevant to the heats of reaction and free energies of amino acids (pp. 33-46). Both of these compilations have since been expanded by additional tables found in later reports. Section I of the present report contains a revision of the heat capacity compilation, and the bibliography to Table 1, NBS Report 8641 contains additional amino acid references.

This first report also contains a preliminary list of compounds of C, H, N, O, P, and S containing not more than one carbon atom per molecule provided by Dr. Morowitz; this list served as the basis for the survey of data given in Table 1, Section II of NBS Report 8595.

For the second quarterly report (NBS Report 8595) the heat capacity data on seventeen amino acids were examined and analyzed by computer, and tabulations were made of molal thermodynamic functions from 0 to 300 °K calculated from the smoothed data (pp. 2-19). This report also contains a table giving selected values of heats of formation, free energies of formation, and entropies available for the compounds on the preliminary list of C, H, N, O, P, and S supplied by Dr. Morowitz, augmented by a few additional compounds (pp. 20-30).

The third quarterly report (NBS Report 8641) contains partial surveys of thermodynamic data (pp. 14-27) and heat capacity data (pp. 1-7) on ubiquitous biochemical compounds and some related compounds. A formula index of the ubiquitous biochemical compounds and related compounds is given on pp. 28-33. The list of ubiquitous compounds was provided by Dr. Morowitz. This report also contains a table (pp. 12-13, with references on pp. 23-27) of selected values of heats of combustion and heats of formation for a number of amino acids and peptides. Two errors in this table should be corrected. The name, L-Isoserine on p. 12

should be DL-isoserine; and the reference for valylphenylalanine on p. 13 is not [67] but is one not listed in the bibliography of the report. The correct reference is Ponomarev, V. V., Alekseeva, T. A., and Akimova, L. N., Zhur. Fiz. Khim. 37, 227-8 (1963).

The present report, like the preceding ones, is divided into two sections, one concerned with the heat capacities, entropies, enthalpies, and free energies of compounds of interest in this survey, and the other dealing with changes in enthalpy and in free energy in reactions of these compounds.

The literature survey in the first section is a revision of the preliminary compilation of heat capacity data for compounds of C, H, N, O, P, and S given in NBS Report 8521, augmented by material given in the second and third progress reports together with a number of additional references.

In the second section, Table 1, giving selected values of heats of combustion and heats of formation for a number of compounds of biological interest, is comparable to the similar table for amino acids and peptides given in NBS Report 8641. The entropies of formation and free energies of formation of fourteen amino acids, given in Table 2 of this section, were calculated using material presented in earlier reports. Table 3 is the supplementary list, mentioned in the previous report (NBS Report 8641, p. 8), of compounds of C, H, N, O, P, and S containing not more than one carbon atom per molecule which were not included in the earlier listing (Table I, p. 20, NBS Report 8595). No specific search for thermodynamic data for compounds on this list has yet been undertaken.

## Section I

### Survey of Heat Capacity, Enthalpy, and Entropy Data on CHNOPS Compounds

Mary K. Buresh and George T. Furukawa

In preparation for a systematic analysis of literature data on thermodynamic properties of CHNOPS compounds, the Chemical Abstracts were searched for heat-capacity data on these substances. The years 1907 to date, except for the half-year period July to December 1964, of the Chemical Abstracts were searched and the original papers examined. Copies of most of the papers have been obtained and cataloged for intensive analysis later.

For this report the substances and their physical states on which thermodynamic data have been found are listed along with the temperature range of the heat measurements. Whenever the data are for solutions, the range of concentrations is given in parentheses immediately below the temperature range of measurements. Pressures are given wherever important. The list includes thermodynamic data given in reviews. The calorimetric entropy at 298°K (or other prescribed temperatures) is given whenever it was calculated by the authors from their data. The entropies of substances in the gaseous state calculated from spectroscopic and molecular data are also listed whenever available. Entropy values given in parentheses are estimates. Whenever the entropy value listed is for a temperature other than 298°K, the following notation is followed:

$$S(\text{phase}, T^{\circ}\text{K}) = \text{value}$$

The unit of entropy used is cal/°K-mol, where 1 calorie = 4.1840 joules.

The substances are cross-referenced to include common names and names approved by the International Union of Chemistry. References to sources of thermodynamic data are listed wherever possible with the names corresponding to those approved by the I. U. C. Whenever the approved name is involved and complicated, the better-known common name is given in parentheses immediately after the I.U.C. approved name. The chemical formula follows these names, except for cases where the composition can not be given precisely.

The kind of heat data contained in the original experimental papers or in reviews is identified by the following:

tc = heat capacity  
tc- = mean heat capacity over relatively broad temperature range  
th = relative enthalpy

The reference numbers in brackets correspond to the bibliography given at the end of this survey. Reviews are indicated by "R". The physical states are identified by:

c = crystal  
l = liquid  
g = gas  
gl = glass



References to  
Heat Capacity, Enthalpy, and Entropy Data on CHNOPS Compounds

<u>Substance</u>	<u>Phase</u>	<u>Year</u>	<u>Temperature Range of Heat Data, °K</u>	<u>Entropy at 298°K cal/°K-mol</u>	<u>References</u>
acetaldehyde: see ethanal					
acetaldehyde, dibutyl acetal: see 1,1-dibutoxyethane					
acetamide: see ethanamide					
acetanilide: see ethanamide, N-phenyl-					
acetanilide, ortho- hydroxy- : see ethanamide, N(2-hydroxyphenyl)-					
acetanilide, meta- hydroxy- : see ethanamide, N(3-hydroxyphenyl)-					
acetanilide, para- hydroxy- : see ethanamide, N(4-hydroxyphenyl)-					
acetanilide, para- nitro- : see ethanamide, N(4-nitrophenyl)-					
acetate, - - -: see ethanoate, - - -					
acetic acid: see ethanoic acid					
acetic acid, amide: see ethanamide					
acetic acid, thiol- : see ethanethiolic acid					
acetone: see 2-propanone					
acetonitrile: see ethanenitrile					
adamantane, 2,4,6,8,9,10-hexathia-, 1,3,5,7-tetramethyl- . $C_8H_{12}S_6$	c, l	1962	tc, 5-347	76.75 (l)	[41]
adamantane, 2,4,6,8-tetrathia-, 1,3,5,7-tetramethyl- . $C_{10}H_{16}S_4$	c, l	1962	tc, 5-346	71.90 (l)	[41]
adenine: see 6-aminopurine					
d-alanine: see l-2-aminopropanoic acid					
dl-alanine: see dl-2-aminopropanoic acid					
l-alanine: see d-2-aminopropanoic acid					
β-alanine: see 3-aminopropanoic acid					
alanine, l-phenyl- : see l-2-amino-3-phenyl- propanoic acid					
allantoin. (5-ureidohydantoin) $NH_2CONH(C_3H_3N_2O_2)$	c	1935	tc, 85-297	46.6 (c)	[242]
alloxan. (pyrimidinetetrone), $NHCONHCOCOO$	c	1935	tc, 86-297	44.6 (c)	[242]
ammonium benzoate: see benzoic acid, ammonium salt					
ammonium cinnamate: see cinnamic acid, ammonium salt					
ammonium cyanide. $NH_4CN$	c	1932	tc, 203-283		[54]
ammonium nitrate. $NH_4NO_3$	c	1865	tc-, 285-321		[139]
	c	1932	tc, 183-273		[54]

Substances	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	References
ammonium oxalate: see ethanedioic acid, ammonium salt					
ammonium orthophosphate, di-H. $\text{NH}_4\text{H}_2\text{PO}_4$	c	1940	tc-, 273-373		[212]
ammonium orthophosphate, mono-H. $(\text{NH}_4)_2\text{HPO}_4$	c	1940	tc-, 273-373		[212]
ammonium phosphate (intermediate salt). $((\text{NH}_4)_3\text{H}_2\text{P}_2\text{O}_8)_x$	c	1940	tc-, 273-373		[212]
ammonium ortho-phthalate: see 1,2-benzenedicarboxylic acid, ammonium salt					
ammonium meta-phthalate: see 1,3-benzenedicarboxylic acid, ammonium salt					
ammonium pyrotartarate, acid: see butanedioic acid, methyl-, ammonium salt					
ammonium succinate: see butanedioic acid, ammonium salt					
ammonium sulfate. $(\text{NH}_4)_2\text{SO}_4$	c	1865	tc-, 286-321		[139]
	c	1932	tc, 183-283		[54]
	c	1945	tc, 53-311	52.6 ±0.3	[231]
ammonium tartarate: see d-2,3-dihydroxybutanedioic acid, ammonium salt					
n-amyl alcohol: see 1-pentanol					
tert-amyl alcohol: see 2-butanol, 2-methyl-					
aniline. (phenylamine), $\text{C}_6\text{H}_5\text{NH}_2$	soln	1899	tc-, 298 (10-60 moles aniline containing 1 mole $\text{H}_2\text{O}$ )		[149]
	c, l	1903	tc-, 251-272		[57]
	l	1928	tc-, 274-332		[140]
	l	1931	tc, 303-413		[32]
	c, l	1933	tc, 94-298	45.8 (l)	[185]
	l	1933	tc, 291-323		[70]
	c, l	1962	tc, 13-313	45.721 (l)	[108]
	g	1962	tc, 298-1000	76.28 (g)	[108]
aniline, N-2,4,6-tetranitro-,N-methyl- : see tetryl					
aniline, ortho- nitro- . (1-amino-2-nitrobenzene), $\text{NO}_2\text{C}_6\text{H}_4\text{NH}_2$	c	1926	tc, 110-333		[10]
aniline, meta- nitro- . (1-amino-3-nitrobenzene), $\text{NO}_2\text{C}_6\text{H}_4\text{NH}_2$	c	1926	tc, 110-344		[10]
	c	1941	tc-, 273-373		[215]
aniline, para- nitro- . (1-amino-4-nitrobenzene) $\text{NO}_2\text{C}_6\text{H}_4\text{NH}_2$	c	1926	tc, 110-344		[10]
	c	1941	tc-, 273-373		[215]
anisic acid: see 4-methoxybenzoic acid					
anisole: see methoxybenzene					
anthranilic acid: see benzoic acid, 2-amino-					
antipyrine. (1,5-dimethyl-2-phenyl-3-pyrazolone), $\text{C}_{11}\text{H}_{12}\text{N}_2\text{O}$	c	1941	tc-, 273-373		[214]
antipyrine, amino- . $\text{C}_{11}\text{H}_{13}\text{N}_3\text{O}$	c	1941	tc-, 273-373		[214]

<u>Substance</u>	<u>Phase</u>	<u>Year</u>	<u>Temperature Range of Heat Data, °K</u>	<u>Entropy at 298°K cal/°K-mol</u>	<u>References</u>
arachidic acid: see eicosanoic acid					
d-arginine: see L-2-amino-5-guanidopentanoic acid					
L-arginine hydrochloride: see d-2-amino-5-guanidopentanoic acid hydrochloride					
L-asparagine: see L-2-aminobutanedioic acid, monoamide					
L-asparagine monohydrate: see L-2-aminobutanedioic acid, monoamide, monohydrate					
L-aspartic acid: see d-aminobutanedioic acid					
3-azabicyclo [3,2,2] nonane, $C_8H_{15}N$	c	1963	tc, 5-345	(56.14) (c)	[21]
2H-azepin-2-one, hexahydro- : see hexanoic acid, 6-amino-, lactam					
azine. (pyridine) $N=CHCH=CHCH=CH$	c, l	1936	tc, 90-300	42.8 (l)	[196]
	c, l	1957	tc, 13-347	42.52 (l)	[154]
azobenzene, 4-amino- . (para-phenylazoaniline) $NH_2C_6H_4N=NC_6H_5$	c	1941	tc-, 273-373		[214]
azobenzene, 2,4-diamino- . (chrysoidine (base)) $(NH_2)_2C_6H_3N=NC_6H_5$	c	1941	tc-, 273-373		[214]
azole. (pyrrole) $NHCHCHCHCH$	g	1957	tc, 300-1000	(S(g,300)=64.97)	[33]
para-azoxybenzoic acid, ethyl ester. $C_2H_5COOC_6H_4NONC_6H_4COOC_2H_5$	c, l	1932	tc, 303-423		[239]
beet sugar: see sucrose					
behenic acid: see docosanoic acid					
1-benzazine. (quinoline), $C_8H_7N=CHCH=CH$	c, l	1936	tc, 90-300	51.9 (l)	[196]
benzene, amino- : see aniline					
benzene, 1,2-dihydroxy- . (catechol, pyrocatechol, pyrocatechin), $C_6H_4(OH)_2$	soln	1901	tc-, 298 (300-400 moles H <sub>2</sub> O containing 1 mole pyrocatechin)		[150]
	c	1926	tc, 110-344		[10]
	c, l	1926	th, 293-473		[11]
	c	1941	tc-, 273-373		[215]
benzene, 1,3-dihydroxy- . (resorcinol, resorcin), $C_6H_4(OH)_2$	soln	1901	tc-, 298 (300-400 moles H <sub>2</sub> O containing 1 mole resorcin)		[150]
	c	1926	tc, 110-344		[10]
	c, l	1926	th, 293-473		[11]
	c	1941	tc-, 273-373		[215]
benzene, 1,4-dihydroxy- . (hydroquinone), $C_6H_4(OH)_2$	soln	1901	tc-, 298 (300-400 moles H <sub>2</sub> O containing 1 mole hydroquinone)		[150]
	c	1924	tc, 28-274		[141]
	c	1926	tc, 110-344		[10]
	soln	1936	tc, 293 (1.5-5.0% aq soln)		[26]
	c	1941	tc-, 273-373		[215]

<u>Substance</u>	<u>Phase</u>	<u>Year</u>	<u>Temperature Range of Heat Data, °K</u>	<u>Entropy at 298°K cal/°K-mol</u>	<u>References</u>
benzene, 1,4-dihydroxy, 2-methyl- . $\text{CH}_3\text{C}_6\text{H}_3(\text{OH})_2$	c	1941	tc-, 273-373		[215]
benzene, 1,2-dinitro- . $\text{C}_6\text{H}_4(\text{NO}_2)_2$	c	1926	tc, 110-344		[10]
benzene, 1,3-dinitro- . $\text{C}_6\text{H}_4(\text{NO}_2)_2$	c	1926	tc, 110-321		[10]
benzene, hydroxy- : see phenol					
benzene, mercapto- : see benzenethiol					
benzene, methoxy- . (anisole) $\text{C}_6\text{H}_5\text{OCH}_3$	l	1959	tc, 363-388		[145]
benzene, 1-methoxy-2-nitro- . (ortho- nitroanisole) $\text{NO}_2\text{C}_6\text{H}_4\text{OCH}_3$	l	1959	tc, 363-408		[145]
benzene, 1-methoxy-3-nitro- . (meta- nitroanisole) $\text{NO}_2\text{C}_6\text{H}_4\text{OCH}_3$	l	1959	tc, 363-408		[145]
benzene, 1-methoxy-4-nitro- . (para- nitroanisole) $\text{NO}_2\text{C}_6\text{H}_4\text{OCH}_3$	l	1959	tc, 363-408		[145]
benzene, methyl- . (toluene) $\text{C}_6\text{H}_5\text{CH}_3$	c, l l	1935 1941	tc, 78-228 tc, 278-320		[12] [263]
benzene, nitro- . $\text{C}_6\text{H}_5\text{NO}_2$	l l	1924 1959	tc, 305-358 tc, 363-408		[259] [145]
benzenecarboxylic acid: see benzoic acid					
1,2-benzenedicarboxylic acid. (phthalic acid) $\text{C}_6\text{H}_4(\text{COOH})_2$	c c	1936 1939	tc, 90-300 tc-, 273-373	49.7 (c)	[196] [211]
1,2-benzenedicarboxylic acid, ammonium salt. $\text{HOOC}\text{C}_6\text{H}_4\text{COONH}_4$	c	1939	tc-, 273-373		[211]
1,2-benzenedicarboxylic acid, ammonium salt. $\text{NH}_4\text{OOC}\text{C}_6\text{H}_4\text{COONH}_4$	c	1939	tc-, 273-373		[211]
1,2-benzenedicarboxylic acid, anhydride. (phthalandione) $\text{C}_6\text{H}_4(\text{CO})_2$	c	1936	tc, 90-300	42.7 (c)	[196]
1,3-benzenedicarboxylic acid. (isophthalic acid) $\text{C}_6\text{H}_4(\text{COOH})_2$	c	1939	tc-, 273-373		[211]
1,3-benzenedicarboxylic acid, ammonium salt. $\text{HOOC}\text{C}_6\text{H}_4\text{COONH}_4$	c	1939	tc-, 273-373		[211]
1,3-benzenedicarboxylic acid, ammonium salt. $\text{NH}_4\text{OOC}\text{C}_6\text{H}_4\text{COONH}_4$	c	1939	tc-, 273-373		[211]
1,4-benzenedicarboxylic acid. $\text{C}_6\text{H}_4(\text{COOH})_2$	c	1941	tc-, 273-373		[216]

<u>Substance</u>	<u>Phase</u>	<u>Year</u>	<u>Temperature Range of Heat Data, °K</u>	<u>Entropy at 298°K cal/°K-mol</u>	<u>Reference</u>
benzenesulfonamide: see benzenesulfonic acid, amide					
benzenesulfonamide, para-amino- : see 4-aminobenzenesulfonic acid, amide					
benzenesulfonic acid, amide. $C_6H_5SO_2NH_2$	c	1941	tc-, 273-373		[214]
benzenesulfonic acid, 4-amino-, amide. (sulfanilamide), $H_2NC_6H_4SO_2NH_2$	c	1941	tc-, 273-373		[214]
benzenethiol. $C_6H_5SH$	c, l c, l	1936 1958	tc, 90-300 tc, 13-375	52.6 (l) 53.25 (l)	[196] [227]
benzenol: see phenol					
benzhydrol: see diphenylmethanol					
benzohydrol: see diphenylmethanol					
benzoic acid. (benzenecarboxylic acid), $C_6H_5COOH$	c, l c l c c, l c, l c c c c, l c	1926 1933 1933 1939 1951 1953 1956 1957 1960 1960 1962	th, 293-473 tc, 93-295  tc-, 273-373 tc, 14-410 tc, 14-410 tc, 80-298 tc, 20-294 tc, 11-303 tc, 4-407 tc, 22-310	 40.8 (c) 49.6 (l)  40.05 (c)  40.11 (c)  40.04 (c)	[11] [185] [185] [211] [80] [92] [201] [55] [46] [236] [138]
benzoic acid, 2-amino- . (anthranilic acid), $NH_2C_6H_4COOH$	c, l c	1926 1941	th, 293-433 tc-, 273-373		[11] [214]
benzoic acid, 3-amino- . $NH_2C_6H_4COOH$	c, l c	1926 1941	th, 293-453 tc-, 273-373		[11] [214]
benzoic acid, 4-amino- . $NH_2C_6H_4COOH$	c, l c	1926 1941	th, 293-463 tc-, 273-373		[11] [214]
benzoic acid, ammonium salt. $C_6H_5COONH_4$	c c	1932 1939	tc, 93-293 tc-, 273-373		[54] [211]
benzoic acid, 2-hydroxy- . (salicylic acid), $HOC_6H_4COOH$	c	1934	tc, 96-289	42.6 (c)	[191]
benzoic acid, 2-hydroxy-, 2-naphthyl ester. $HOC_6H_4COOC_{10}H_7$	c, l gl, l	1910 1910	th, 83-350 th, 82-362		[170] [170]
benzoic acid, 3-hydroxy- . $HOC_6H_4COOH$	c	1934	tc, 94-288	42.3 (c)	[191]
benzoic acid, 4-hydroxy- . $HOC_6H_4COOH$	c	1934	tc, 95-284	42.0 (c)	[191]
benzoic acid, 4-methoxy- . (anisic acid), $CH_3OC_6H_4COOH$	c	1941	tc-, 273-373		[215]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
benzoic acid, 2-methyl- $\text{CH}_3\text{C}_6\text{H}_4\text{COOH}$	c, l	1926	th, 293-473		[11]
benzoic acid, 3-methyl- $\text{CH}_3\text{C}_6\text{H}_4\text{COOH}$	c, l	1926	th, 293-443		[11]
benzoic acid, 4-methyl- $\text{CH}_3\text{C}_6\text{H}_4\text{COOH}$	c, l	1926	th, 293-498		[11]
benzoic acid, 2-nitro- $\text{NO}_2\text{C}_6\text{H}_4\text{COOH}$	c c	1926 1941	tc, 110-344 tc-, 273-373		[10] [213]
benzoic acid, 3-nitro- $\text{NO}_2\text{C}_6\text{H}_4\text{COOH}$	c c	1926 1941	tc, 110-344 tc-, 273-373		[10] [213]
benzoic acid, 4-nitro- $\text{NO}_2\text{C}_6\text{H}_4\text{COOH}$	c c	1926 1941	tc, 110-344 tc-, 273-373		[10] [213]
benzophenone. (phenyl ketone) $(\text{C}_6\text{H}_5)_2\text{CO}$	gl, l c, l c	1910 1910 1925	th, 80-314 th, 80-314 th, 89-290		[170] [170] [146]
1,4-benzoquinone. $\text{OC}_6\text{H}_4\text{O}$	c c, l	1924 1926	tc, 22-291 th, 293-433		[141] [11]
benzothiophene: see thiophene, 2,3-benzo-					
benzyl alcohol. (phenylcarbinol) $\text{C}_6\text{H}_5\text{CH}_2\text{OH}$	c, l c, l	1931 1936	tc, 102-299 tc, 90-300	51.8 (l)	[237] [196]
poly-γ-benzyl-L-glutamate: see poly-γ-benzyl-D-2-aminopentanedioic acid					
bstol: see benzoic acid, 2-hydroxy-, 2-naphthyl ester					
bicyclo [2,2,1] heptane, endo-2-cyano- $\text{C}_7\text{H}_{11}\text{CN}$	c, l	1962	tc, 12-350	53.49 ± 0.25	[230]
bicyclo [2,2,1] heptane, exo-2-cyano- $\text{C}_7\text{H}_{11}\text{CN}$	c, l	1962	tc, 12-350	55.11 ± 0.26	[230]
bicyclo [3,2,2] nonane, 3-aza- : see 3-azabicyclo [3,2,2] nonane					
bicyclo [2,2,2] octane, 1,4-diaza- : see triethylenediamine					
bovine serum albumin, anhydrous: see serum albumin, bovine, anhydrous					
bovine serum albumin, hydrated: see serum albumin, bovine, hydrated					
1,3-butadiene, 1,4-epoxy- . (furan), $\text{OCHCHCHCH}$	c, l g	1952 1957	tc, 12-300 tc, 300-1000	42.22 ± 0.08 (l) 63.86 ± 0.10 (g) (S(g, 304.5) = 64.34)	[105] [33]
1,3-butadiene, 1,4-epoxy-, 2-methyl- $\text{C}_4\text{H}_3\text{OCH}_3$	c, l	1962	tc, 7-307	51.118 (l)	[38]
1,3-butadiene, 2-methyl- . (isoprene) $\text{CH}_2\text{CHC}(\text{CH}_3)\text{CH}_2$	c, l	1937	tc, 23-298	229.3 ± 1.0 (J/deg-mole)	[25]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
butanal. (butyraldehyde) $\text{CH}_3(\text{CH}_2)_2\text{CHO}$	c, l	1956	tc, 80-300	59.0 (l)	[190]
butane, 2,3-dithia- $(\text{CH}_3\text{S})_2$	c, l	1950	tc, 13-352	56.26 ± 0.10 (l)	[219]
	g	1958	tc, 369-500	80.54 ± 0.30 (g)	
				80.46 (g)	
				$S(g, 340.80) = 83.57$ $S(l, 360.40) = 63.03$ $S(g, 360.40) = 84.91$ $S(g, 382.90) = 86.44$	
butane, 2-thia- $\text{CH}_3\text{SC}_2\text{H}_5$	c, l	1951	tc, 14-298	57.14 ± 0.10 (l)	[223]
	g	1959		79.62 (g)	[226]
butane, 2-thia-, 3,3-dimethyl- (methyl t-butyl sulfide) $\text{CH}_3\text{SC}(\text{CH}_3)_2\text{CH}_3$	c, l	1962	tc, 15-364	66.00 (l)	[225]
	g	1962	tc, 273-1000	89.21 (g)	[225]
butane, 2-thia-, 3-methyl- $\text{CH}_3\text{SCH}(\text{CH}_3)_2$	c, l	1955	tc, 13-344	62.88 ± 0.12 (l)	[157]
butanedinitrile. (succinonitrile), $\text{CNCH}_2\text{CH}_2\text{CN}$	c, l	1963	tc, 5-348	45.79 (c)	[260]
	g	1963		79.04 ± 0.10 (g)	[260]
butanedioic acid. (succinic acid), $\text{COOH}(\text{CH}_2)_2\text{COOH}$	c	1865	tc-, 292-324		[139]
	c	1930	tc, 93-290	42.0 (c)	[184]
	c	1938		42.0 (c)	[117]
	c	1939	tc-, 273-373		[210]
butanedioic acid, d-amino- (l-aspartic acid) $\text{HOOCCH}_2(\text{NH}_2)\text{CHCOOH}$	c	1932	tc, 88-294	41.5 (c)	[113]
	c	1963	tc, 11-301	40.66 (c)	[120]
	c	1964	tc, 0-300	40.657 (c)	[13 R]
butanedioic acid, l-2-amino-, monoamide. (l-asparagine) $\text{NH}_2\text{COCH}_2\text{CH}(\text{NH}_2)\text{COOH}$	c	1932	tc, 85-297	41.7 (c)	[113]
butanedioic acid, l-2-amino-, monoamide, monohydrate. $\text{NH}_2\text{COCH}_2(\text{NH}_2)\text{CHCOOH} \cdot \text{H}_2\text{O}$	c	1932	tc, 90-297	51.0 (c)	[113]
	c	1963	tc, 11-303	50.10 (c)	[120]
	c	1964	tc, 0-300		
			th, 0-300	50.103 (c)	[13 R]
butanedioic acid, ammonium salt. $\text{HOOC}(\text{CH}_2)_2\text{COONH}_4$	c	1939	tc-, 273-373		[210]
butanedioic acid, ammonium salt. $\text{NH}_4\text{OOC}(\text{CH}_2)_2\text{COONH}_4$	c	1939	tc-, 273-373		[210]
butanedioic acid, diamide. (succinamide) $\text{NH}_2\text{COCH}_2\text{CH}_2\text{CONH}_2$	c	1941	tc-, 273-373		[216]
butanedioic acid, dl-2,3-dihydroxy- (dl-tartaric acid) $\text{HOOC}(\text{CHOH})_2\text{COOH} \cdot \text{H}_2\text{O}$	c	1865	tc-, 292-324		[139]
butanedioic acid, d-2,3-dihydroxy- $\text{HOOC}(\text{CHOH})_2\text{COOH}$	c	1865	tc-, 293-324		[139]
	c	1906	tc, 83-287		[75]
	c	1914	tc, 83-328		[67]
	c	1939	tc-, 273-373		[210]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	References
butanedioic acid, d-2,3-dihydroxy-, ammonium salt. $\text{HOOC}(\text{CHOH})_2\text{COONH}_4$	c	1939	tc-, 273-373		[210]
butanedioic acid, d-2,3-dihydroxy-, ammonium salt. $\text{NH}_4\text{OOC}(\text{CHOH})_2\text{COONH}_4$	c	1939	tc-, 273-373		[210]
butanedioic acid, d-2,3-dihydroxy-, diethyl ester. $\text{C}_2\text{H}_5\text{OOCCHOHCHOHCOOC}_2\text{H}_5$	l	1930	tc-, 299-372		[255]
butanedioic acid, meso-2,3-dihydroxy-, diethyl ester. $\text{C}_2\text{H}_5\text{OOCCHOHCHOHCOOC}_2\text{H}_5$	c, l	1930	tc-, 260-372		[255]
butanedioic acid, l-hydroxy- . (l-malic acid) $\text{HOOCCH}(\text{OH})\text{CH}_2\text{COOH}$	c	1931		49. (c)	[34]
butanedioic acid, imide. (succinimide) $(\text{CH}_2\text{CO})_2\text{NH}$	c	1941	tc-, 273-373		[216]
butanedioic acid, methyl- . $\text{COOHCH}_2\text{CH}(\text{CH}_3)\text{COOH}$	c	1939	tc-, 273-373		[210]
butanedioic acid, methyl-, ammonium salt. $\text{HOOCCH}_2\text{CH}(\text{CH}_3)\text{COONH}_4$	c	1939	tc-, 273-373		[210]
1,2,3,4-butanetetrol. (erythritol) $(\text{CH}_2\text{OHCHOH})_2$	c c c, l	1926 1929 1932	tc, 87-292 tc, 303-423	42.5 (c) 39.8 ±.4 (c)	[181] [189] [239]
1-butanethiol. (n-butylmercaptan) $\text{CH}_3(\text{CH}_2)_2\text{CH}_2\text{SH}$	c, l	1957	tc, 13-314	65.96 (l)	[224]
2-butanethiol. (isobutylmercaptan) $\text{CH}_3\text{CHSHCH}_2\text{CH}_3$	c, l	1958	tc, 12-307	64.87 (l) 87.67 (g)	[159]
2-butanethiol, 2-methyl- . (tert-amyl mercaptan) $\text{CH}_3\text{C}(\text{CH}_3)(\text{SH})\text{CH}_2\text{CH}_3$	c, l g	1962 1962	tc, 12-347 tc, 0-1000	69.34 (l) 92.48 (g)	[218] [218]
butanoic acid. (butyric acid) $\text{CH}_3\text{CH}_2\text{CH}_2\text{COOH}$	c, l c	1926 1929	tc, 89-291	61.0 (l) 54.1 ±.5 (c)	[181] [189]
butanoic acid, 2-amino- . (α-aminobutyric acid) $\text{CH}_3\text{CH}_2\text{CH}(\text{NH}_2)\text{COOH}$	c	1941	tc-, 273-373		[215]
butanoic acid, l-2-amino-, 3-hydroxy- . (l-threonine) $\text{CH}_3\text{CHOH}(\text{NH}_2)\text{CHCOOH}$	c	1964	tc, 10-310		[119]
butanoic acid, d-2-amino-3-methyl- . (l-valine) $(\text{CH}_3)_2\text{CH}(\text{NH}_2)\text{CHCOOH}$	c c	1963 1964	tc, 11-301 tc, 0-300	42.75 (c) 42.719 (c)	[122] [13 R]
butanoic acid, dl-2-amino-3-methyl- . (dl-valine) $(\text{CH}_3)_2\text{CHCH}(\text{NH}_2)\text{COOH}$	soln	1935	tc, 298 (0-0.63 molal)		[264]



Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
butanoic acid, L-2-amino-, 4-(methylthio)-. (L-methionine) $\text{CH}_3\text{SCH}_2\text{CH}_2\text{CH}(\text{NH}_2)\text{COOH}$	c	1964	tc, 11-348	55.32 (c)	[124]
butanoic acid, 3-methyl-, ethyl ester. (ethyl isovalerate) $(\text{CH}_3)_2\text{CHCH}_2\text{COOC}_2\text{H}_5$	l	1949	tc, 313-343		[143]
1-butanol. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$	l	1924	tc, 307-348		[259]
	c, l	1925	tc, 91-294	60.2 (l)	[180]
	l	1929		54.5 ± .5 (l)	[189]
	g	1938	tc, 410		[27]
	g	1950	tc, 408-435 (760 mm pressure)		[204]
	g	1953	tc, 394-437 (750 mm pressure)		[234]
	g	1962	tc, 365-455	85.81 (g)	[30]
1-butanol, 2-methyl. (sec-butyl carbinol) $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{OH}$	l	1949	tc, 313-343		[143]
1-butanol, 3-methyl-. $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{OH}$	l	1924	tc, 314-353		[259]
	l	1949	tc, 313-343		[143]
	l	1958	tc-, 295-400		[247]
	l	1958	tc-, 295-400		[248]
2-butanol. $\text{CH}_3\text{CH}_2\text{CHOHCH}_3$	gl, l	1936	tc, 103-282		[195]
	g	1950	tc, 409-431 (760 mm pressure)		[204]
	g	1953	tc, 375-437 (750 mm pressure)		[234]
2-butanol, 2-methyl. (tert-amyl alcohol) $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)\text{OHCH}_3$	c, l	1933	tc, 92-294	54.8 (l)	[185]
	l	1949	tc, 313-343		[143]
2-butanone. (ethyl methyl ketone) $\text{CH}_3\text{COC}_2\text{H}_5$	g	1938	tc, 410		[27]
	c, l	1956	tc, 80-300	57.7 (l)	[190]
	l	1961		58.72 (l)	[172]
	g	1961	tc, 347-467	82.51 (g)	[172]
	c, l	1964	tc, 13-338	57.08 (l)	[235]
	g	1964		80.81 (g)	[235]
cis-butenedioic acid. (maleic acid) $\text{HOOCCH=CHCOOH}$	c	1930	tc, 91-294	38.1 (c)	[184]
	c	1938		38.1 (c)	[117]
cis-butenedioic acid, dimethyl ester. (methyl maleate) $\text{CH}_3\text{OOCCH=CHCOOCH}_3$	l	1930	tc-, 273-372		[254]
trans-butenedioic acid. (fumaric acid) $\text{HOOCCH=CHCOOH}$	c	1930	tc, 91-297	39.7 (c)	[184]
	c	1938		39.7 (c)	[117]
trans-butenedioic acid, dimethyl ester. $\text{CH}_3\text{OOCCH=CHCOOCH}_3$	c	1930	tc-, 259-372		[254]
n-butyl alcohol: see 1-butanol					
sec-butyl alcohol: see 2-butanol					
tert-butyl alcohol: see 2-methyl-2-propanol					

<u>Substance</u>	<u>Phase</u>	<u>Year</u>	<u>Temperature Range of Heat Data, °K</u>	<u>Entropy at 298°K cal/°K-mol</u>	<u>Reference</u>
n-butyl carbinol: see 1-pentanol					
sec-butyl carbinol: see 1-butanol, 2-methyl-					
butyraldehyde: see butanal					
butyric acid: see butanoic acid					
cane sugar: see sucrose					
capric acid: see decanoic acid					
caproic acid: see hexanoic acid					
ε-caprolactam: see hexanoic acid, 6-amino-, lactam					
poly-ε-caprolactam: see poly-hexanoic acid, 6-amino-, lactam					
caprylic acid: see octanoic acid					
carbinol, n-butyl- : see 1-pentanol					
carbinol, sec-butyl- : see 1-butanol, 2-methyl-					
carbinol, diethyl- : see 3-pentanol					
carbinol, di-methyl ethyl- : see 2-butanol, 2-methyl-					
carbinol, diphenyl- : see diphenylmethanol					
carbinol, isobutyl- : see 3-methyl-1-butanol					
carbinol, triphenyl- . $(C_6H_5)_3COH$	c	1931	tc, 102-346		[237]
catechol: see 1,2-dihydroxybenzene					
cerotic acid: see hexacosanoic acid					
cetyl alcohol: see 1-hexadecanol					
chymotrypsinogen, anhydrous. c		1964	tc, 10-310		[119]
chymotrysinogen, hydrated. c		1964	tc, 10-310		[119]
cinnamic acid. $C_6H_5CH:CHCOOH$	c	1939	tc-, 273-373		[211]
cinnamic acid, 3-amino- . $NH_2C_6H_4CH:CHCOOH$	c	1941	tc-, 273-373		[214]
cinnamic acid, ammonium salt. $C_6H_5CH:CHCOONH_4$	c	1939	tc-, 273-373		[211]
cinnamic acid, 2-nitro- . $NO_2C_6H_4C_2H_2COOH$	c	1941	tc-, 273-373		[213]
cinnamic acid, 3-nitro- . $NO_2C_6H_4C_2H_2COOH$	c	1941	tc-, 273-373		[213]
cinnamic acid, 4-nitro- . $NO_2C_6H_4C_2H_2COOH$	c	1941	tc-, 273-373		[213]
citric acid monohydrate: see 2-hydroxy-1,2,3-propanetricarboxylic acid monohydrate					
dl-citrulline. (dl-α-amino-δ-ureidovaleric acid) $NH_2CONH(CH_2)_3(NH_2)CHCOOH$	c	1940	tc, 89-301	60.8 (c)	[118]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
cottonseed oil.	l	1944	tc-, 318-373		[104]
cottonseed stearine.	c, l	1944	tc-, 273-373		[104]
cream, ripe.	l	1959	tc, 280-324		[252]
creatine. (( $\alpha$ -methylguanido) acetic acid) $\text{NH}_2\text{C}(=\text{NH})\text{N}(\text{CH}_3)\text{CH}_2\text{COOH}$	c	1932	tc, 87-296	45.3 (c)	[113]
	c	1941	tc-, 273-373		[215]
creatine hydrate. ( $\alpha$ -methylguanido) acetic acid hydrate $(\text{NH}_2)\text{C}(=\text{NH})\text{N}(\text{CH}_3)\text{CH}_2\text{COOH}\cdot\text{H}_2\text{O}$	c	1940	tc, 87-298	56.0 (c)	[118]
creatinine. (1-methylglycocycamidine) $\text{CH}_3\text{NC}(=\text{NH})\text{NHCOCH}_2$	c	1932	tc, 87-296	40.0 (c)	[113]
endo-2-cyanobicyclo [2.2.1] heptane: see bicyclo [2,2,1] heptane, endo-2-cyano-					
exo-2-cyanobicyclo [2.2.1] heptane: see bicyclo [2,2,1] heptane, exo-2-cyano-					
cyanogen: see ethanedinitrile					
cyclobutane, thia- . $(\text{CH}_2)_3\text{S}$	c, l	1953	tc, 12-321	44.72 $\pm$ 0.10 (l) 68.17 $\pm$ 0.25 (g)	[220]
cyclohexane, thia- . $(\text{CH}_2)_5\text{S}$	c, l	1954	tc, 13-342	52.16 $\pm$ 0.10 (l)	[155]
cyclohexanol. $\text{C}_6\text{H}_{11}\text{OH}$	c, l	1929	tc, 15-299	47.8 $\pm$ 0.3 (l) I 47.5 $\pm$ 0.3 (l) II	[133]
cyclopentane, thia- . $(\text{CH}_2)_4\text{S}$	c, l	1952	tc, 13-333	49.67 $\pm$ 0.10 (l)	[111]
cyclopentanethiol. $\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{SH}$ $\text{[CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{]}$	c, l	1961	tc, 12-366	61.39 (l)	[28]
cyclopentanol. $\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CHOH}$ $\text{[CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{]}$	c, l	1956	tc, 80-300	49.3 (l)	[190]
l-cysteine: see l-2-amino-3-mercaptopropanoic acid					
l-cystine: see l-3,3'-dithiobis (2-aminopropanoic acid)					
decanoic acid. (capric acid) $\text{CH}_3(\text{CH}_2)_8\text{COOH}$	c, l	1924	tc-, 273-338		[84]
n-decoic acid: see decanoic acid					
dextrose: see d-glucose					
diglycine: see glycylglycine					
dilactic acid, $\beta,\beta'$ -dithio- . ( $\beta,\beta'$ -dithiodilactic acid) $(\text{CH}_2\text{CHSHCOOH})_2$	c	1935	tc, 85-305	65.5 (c)	[114]
dimethylamine. $(\text{CH}_3)_2\text{NH}$	g	1933	tc, 283-323		[69]
	c, l	1939	tc, 14-280	43.58 $\pm$ 0.05 (l) $S^\circ(1,280.04)=41.55$	[15]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
dimethyl formamide: see methanamide, dimethyl-					
dimethyl sulfide: see thiapropane					
dimethyl sulfone: see methyl sulfone					
dimethyl sulfoxide: see methyl sulfoxide					
1,4-dioxane. (diethylene dioxide) $\text{OCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2$	c, l soln	1934 1936	tc, 93-298 tc, 293 (2-10% aq soln)	47.0 (l)	[127] [26]
diphenyl ether: see phenyl ether					
diphenyl oxide: see phenyl ether					
diphenylsulfide. (phenylthiobenzene) $(\text{C}_6\text{H}_5)_2\text{S}$	c, l	1931	tc, 102-299		[238]
diphenylsulfone. (phenylsulfonylbenzene) $(\text{C}_6\text{H}_5)_2\text{SO}_2$	c	1931	tc, 102-346		[238]
diphenylsulfoxide. $(\text{C}_6\text{H}_5)_2\text{SO}$	c	1931	tc, 102-323		[238]
1,3-bis-diphenylene-2-phenyl allyl. $\text{C}_{12}\text{H}_8\text{C}_6\text{H}_5\text{CH}_2\text{CHCH}_2$	c	1963	tc, 1.3-7.0		[107]
docosanoic acid. (behenic acid) $\text{CH}_3(\text{CH}_2)_{20}\text{COOH}$	c, l	1929	tc-, 291-382		[82]
dodecanoic acid. (lauric acid) $\text{CH}_3(\text{CH}_2)_{10}\text{COOH}$	c, l l	1924 1930	tc-, 291-351 tc-, 367-529		[84] [142]
dulcite: see 1,2,3,4,5,6- hexanehexol (dulcitol)					
dulcitol: see 1,2,3,4,5,6-hexanehexol					
eicosanoic acid. (arachidic acid) $\text{CH}_3(\text{CH}_2)_{18}\text{COOH}$	c, l	1926	tc-, 293-373		[83]
n-eicosoic acid: see eicosanoic acid					
enanthaldehyde: see heptanal					
enanthic acid: see heptanoic acid					
ε-enantholactam. (2(lH)-azocinone, hexahydro) $\text{C}_7\text{H}_{13}\text{NO}$	c, l c, l	1959 1962	tc, 60-350 tc, 62-350	45.4 (c) 45.4 ± 0.5 (c)	[137] [136]
poly-ε-enantholactam. (poly-2(lH)-azocinone, hexahydro) $(\text{C}_7\text{H}_{13}\text{NO})_x$	c	1962	tc, 63-350	49.4 ± 0.5 (c)	[136]
1,2-epoxyethane. $(\text{CH}_2)_2\text{O}$	g c, l	1940 1949	tc-, 307-371 tc, 15-284	$\text{S}^\circ(\text{l}, 283.60) = 35.72$ $\text{S}^\circ(\text{g}, 283.60) = 57.38$	[135] [86]
erythritol: see 1,2,3,4-butanetetrol					
ethanal. (acetaldehyde) $\text{CH}_3\text{CHO}$	l g	1947 1949	tc-, 273 tc, 299-422		[51] [49]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
ethanamide. (acetamide) $\text{CH}_3\text{CONH}_2$	soln	1899	tc-, 298 (100-200 moles $\text{H}_2\text{O}$ con- taining 1 mole acetamide)		[149]
ethanamide, 2-hydroxy- . (glycolamide) $\text{CH}_2\text{OHCONH}_2$	soln	1939	tc, 278-313 (0-2.3 molarity)		[102]
	soln	1941	tc, 278-313 (3.4952-4.5282 molarity)		[101]
ethanamide, N(2-hydroxyphenyl)- . (2-acetaminophenol) $\text{CH}_3\text{CONHC}_6\text{H}_4\text{OH}$	c, l	1926	th, 323-413		[11]
ethanamide, N(3-hydroxyphenyl)- . (3-acetaminophenol) $\text{CH}_3\text{CONHC}_6\text{H}_4\text{OH}$	c, l	1926	th, 323-413		[11]
ethanamide, N(4-hydroxyphenyl)- . (4-acetaminophenol) $\text{CH}_3\text{CONHC}_6\text{H}_4\text{OH}$	c, l	1926	th, 323-413		[11]
ethanamide, N(4-nitrophenyl)- . (para-nitroacetanilide) $\text{CH}_3\text{CONHC}_6\text{H}_4\text{NO}_2$	c	1941	tc-, 273-373		[213]
ethanamide, N-phenyl. (acetanilide) $\text{CH}_3\text{CONHC}_6\text{H}_5$	c	1941	tc-, 273-373		[213]
ethane, dibenzoyl- . $\text{C}_6\text{H}_5\text{CO}(\text{CH}_2)_2\text{OCC}_6\text{H}_5$	c, l	1932	tc, 303-463		[239]
ethane, 1,1-dibutoxy- . (acetaldehyde, dibutyl acetal) $\text{CH}_3\text{CH}(\text{OC}_4\text{H}_9)_2$	l	1947	tc-, 298-353		[51]
ethane, 1,2-epoxy- : see 1,2-epoxyethane					
ethanedinitrile. (cyanogen) $\text{NCCN}$	g	1936	tc, 173-279		[65]
	c, l	1939	tc, 15-252	(57.64) (g) $S^\circ(l, 251.95) = 33.19$	[206]
	g	1939	tc, 273-327		[37]
	g	1939	tc, 185-320		[243]
ethanedioic acid. (oxalic acid) $\text{HOOCOOH}$	c	1910	tc, 84-202		[168]
	c	1910	th, 84-273		[170]
	c	1911	tc, 84-202		[169]
	c	1925		30.4 (c)	[187]
	c	1929		28.7 ± 0.3 (c)	[189]
	c	1939	tc-, 273-373		[210]
ethanedioic acid, ammonium salt. (acid ammonium oxalate) $\text{HOOC(OONH)}_4$	c	1932	tc, 183-283		[54]
	c	1939	tc-, 273-373		[210]
ethanedioic acid, ammonium salt. (diammonium oxalate) $\text{H}_2\text{NOOC(OONH)}_4$	c	1939	tc-, 273-373		[210]
ethanedioic acid, diethyl ester. $(\text{COOC}_2\text{H}_5)_2$	l	1949	tc, 313-343		[143]
ethanedioic acid dihydrate. $\text{HOOCOOH} \cdot 2\text{H}_2\text{O}$	c	1910	tc, 84-198		[168]
	c	1910	th, 82-273		[170]
	c	1911	tc, 84-198		[169]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K mol	Reference
1,2-ethanediol. <chem>CH2OHCH2OH</chem>	c, l c, l l soln	1901 1925 1929 1932	th, 250-412 tc, 88-293  tc, 293-352 (25-100% glycol)	 42.9 (l) 39.9 ±.4 (l)	[56] [187] [189] [166]
ethanenitrile. (acetonitrile) <chem>CH3CN</chem>	c, l	1965	tc, 16-301	35.76 ±0.15 (l) 58.67 ±0.20 (g) [203]	
ethanesulfonic acid, 2-amino- : see taurine					
ethanethiol. (ethyl mercaptan) <chem>CH3CH2SH</chem>	c, l	1952	tc, 14-315	49.48 ±0.10 (l) 70.77 ±0.15 (g) [160]	
ethanethiolic acid. (thiolacetic acid) <chem>CH3COSH</chem>	g	1963	tc, 273.15-1000	74.86 (g)	[148]
ethanoate, ethyl. <chem>CH3COOC2H5</chem>	c, l g	1933 1938	tc, 92-294 tc, 410	62.0 (l)	[185] [27]
ethanoate, methyl. <chem>CH3COOCH3</chem>	g	1938	tc, 410		[27]
ethanoate, β-methylpropyl- . <chem>CH3COOCH2CH(CH3)2</chem>	g	1938	tc, 410		[27]
ethanoic acid. (acetic acid) <chem>CH3COOH</chem>	c c c, l c soln soln soln g	1903 1913 1925 1929 1932 1932 1958 1958	tc-, 251-286 tc-, 20- 80 tc, 87-275  tc, 297-354 (5.44-100% <chem>CH3COOH</chem> ) tc, 297-354 (5.44-100% <chem>CH3COOH</chem> ) tc, 273-393 (0.503-2.998 mol/kg-H <sub>2</sub> O)	  46.3 (l) 38.2 ±0.4 (c)	[57] [61] [187] [189] [165] [171] [2] [2]
ethanoic acid, amino- . (glycine) <chem>NH2CH2COOH</chem>	c soln soln soln c c	1933 1935 1939 1940 1960 1964	tc, 93-300 tc, 298 (0-3.33 molal) tc, 278-313 (0-2.7 molarity)  tc, 12-302 tc, 0-300 th, 0-300	26.1 (c)  40.5 (1 molal solution) 24.74 (c)	[185] [264] [102] [103] [121] [13 R]
ethanoic acid, amino-, dl-alanyl- . (dl-alanylglycine) <chem>(H2N)(CH3)CHCONHCH2COOH</chem>	c	1941	tc, 85-296	51.0 (c)	[112]
ethanoic acid, amino-, N-benzoyl- : see hippuric acid					
ethanoic acid, amino-, glycy- : see glycyglycine					
ethanoic acid, ethyl ester: see ethanoate, ethyl					
ethanoic acid, hydroxy-(phenyl)- . (mandelic acid) <chem>C6H5CH(OH)COOH</chem>	c	1941	tc-, 273-373		[215]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298° cal/°K mol	Reference
ethanoic acid, isobutyl ester: see $\beta$ -methylpropyl ethanoate					
ethanoic acid, methyl ester: see methyl ethanoate					
ethanoic acid, nitrile: see ethanenitrile					
ethanoic acid, thiol- : see ethanethiolic acid					
ethanoic acid dimer. $(\text{CH}_3\text{COOH})_2$	g	1959		$S(g, 373) = 22.26$	[164]
ethanol. $\text{CH}_3\text{CH}_2\text{OH}$	l	1907	tc-, 182-245		[22]
	l	1907	tc-, 278-315		[35]
	l	1908	tc, 182-245		[23]
	gl	1920	tc, 86-96		[90]
	c	1920	tc, 88-141		[90]
	l	1920	tc, 196-271		[90]
	l	1924	tc, 300-330		[259]
	gl	1925	tc, 87-110		[180]
	c, l	1925	tc, 87-298	42.3 (l)	[180]
	gl, l	1927	tc, 87-298		[183]
	gl, l	1929	tc, 18-108		[131]
	gl	1929		$S^\circ(g, 1, 0) = 2.6$	[131]
	gl, l	1929		$S^\circ(l, 298) - S^\circ(g, 1, 0)$ $= 35.8$	[131]
	c, l	1929	tc, 19-294	38.4 $\pm 0.3$ (l)	[131]
	l	1929	tc, 184-269		[163]
	l	1929		38.4 $\pm 0.4$ (l)	[189]
	g	1938	tc, 410		[27]
	g	1953	tc, 354-437		
			(pressure 750 mm)		[234]
	c, l	1961	tc, 16-350	38.53 (l)	[96 R]
	g	1961	tc, 273-1000	67.54 (g)	[96 R]
ethanol-water mixture. $\text{CH}_3\text{CH}_2\text{OH}-\text{H}_2\text{O}$	soln	1899	tc-, 298 (12.5-300 moles $\text{H}_2\text{O}$ containing 1 mole alcohol)		[149]
	soln	1907	tc-, 273-316 (0-100% alcohol by weight)		[35]
	soln	1931	tc, 303-348 (25-100% alcohol by weight)		[32]
	soln	1931	th, 313-383 (192 volume proof)		[73]
	soln	1931	th, 287-380 (concentration: 3.0-90.3 kg/kg- $\text{H}_2\text{O}$ )		[36]
	soln	1932	tc, 273-361 (2.5-100% $\text{C}_2\text{H}_5\text{OH}$ )		[245]
	mixt, g	1961	tc, 461-645 (74%, 75-250 atm pressure)		[205]
ethanol-1-propanol (equimolar mixture). $\text{C}_2\text{H}_5\text{OH}-\text{C}_3\text{H}_7\text{OH}$	gl, l	1920	tc, 78-273		[90]
ethanol, 2-amino- . (ethanolamine) $\text{NH}_2\text{CH}_2\text{CH}_2\text{OH}$	soln	1955	tc, 278-433 (8-25% aq solution)		[43]
ethanolamine: see ethanol, 2-amino-					
ethoxyethane. (ethyl ether) $\text{C}_2\text{H}_5\text{OC}_2\text{H}_5$	l	1907	tc-, 182-252		[22]
	c, l	1926	tc, 76-290	67.7 (l)	[182]
	c	1929		60.4 $\pm 0.6$ (l)	[189]
	c, l	1935	tc, 80-255		[12]

<u>Substance</u>	<u>Phase</u>	<u>Year</u>	<u>Temperature Range of Heat Data, °K</u>	<u>Entropy at 298° cal/°K mol</u>	<u>Reference</u>
ethyl acetate: see ethyl ethanoate					
ethyl alcohol: see ethanol					
ethyl ether: see ethoxyethane					
ethyl formate: see ethyl methanoate					
ethyl isovalerate: see 3-methylbutanoic acid, ethyl ester					
ethyl nitrate. (nitric ether) $C_2H_5ONO_2$	c, l	1954	tc, 22-293	59.08 (l)	[95]
ethyl oxalate: see ethanedioic acid, diethyl ester					
ethyl propionate: see propanoic acid, ethyl ester					
ethyl valerate: see pentanoic acid, ethyl ester					
ethylene glycol: see 1,2-ethanediol					
ethylene oxide: see 1,2-epoxyethane					
formamide: see methanamide					
formic acid: see methanoic acid					
d-fructose. (levulose) $C_6H_{12}O_6$	soln	1901	tc-, 298 (201.5-400 moles $H_2O$ containing 1 mole sugar)		[150]
fumaric acid: see trans-butenedioic acid					
furan: see 1,4-epoxy-1,3-butadiene					
2-furancarbal. (furfural) $C_4H_3OCHO$	l	1962	tc, 288-422		[177]
furfural: see 2-furancarbal.					
furfuryl alcohol. (2-furancarbinol) $C_4H_3OCH_2OH$	c, l	1956	tc, 90-300	51.6 (l)	[190]
galactitol: see 1,2,3,4,5,6-hexanehexol					
$\alpha$ -d-galactose. $C_6H_{12}O_6$	c	1941	tc, 64-297	49.1 (c)	[126]
d-glucose. (dextrose) $C_6H_{12}O_6$	c	1922	tc, 20-296		[232]
	c	1925		53.4 (c)	[187]
	gl, l	1928	tc, 94-340		[186]
	c	1929		50.5 $\pm$ 0.5 (c)	[189]
	gl, l	1934	tc, 255-319		[193]
	gl	1941	th, 273-333		[167]
	c	1951	th, 273-363		[62]
d-glucose — water system. $C_6H_{12}O_6 - H_2O$	soln	1899	tc-, 298 (100-300 moles $H_2O$ containing 1 mole sugar)		[149]
	soln	1935	tc, 289-312 (0.25-1.00 gm-mole/kg- $H_2O$ )		[77]
	soln	1936	tc, 293 (5-10% aq soln)		[26]
	soln	1955	tc, 298 (0.1-8.4 molal)		[250]



<u>Substance</u>	<u>Phase</u>	<u>Year</u>	<u>Temperature Range of Heat Data, °K</u>	<u>Entropy at 298° cal/°K mol</u>	<u>Reference</u>
$\alpha$ -d-glucose. $C_6H_{12}O_6$	c c	1934 1938	tc, 263-333	50.7 (c)	[193] [117]
$\alpha$ -d-glucose hydrate. $C_6H_{12}O_6 \cdot H_2O$	c	1938		(60.4)	[117]
$\beta$ -d-glucose. $C_6H_{12}O_6$	c	1938		(54.4)	[117]
d-glutamic acid: see l-2-aminopentanedioic acid					
d-glutamic acid hydrochloride: see l-2-aminopentanedioic acid hydrochloride					
l-glutamic acid: see d-2-aminopentanedioic acid					
l-glutamine. (d- $\alpha$ -aminoglutaramic acid) $NH_2CO(CH_2)_2(NH_2)CHCOOH$	c c	1963 1964	tc, 11-308 tc, 0-300 th, 0-300	46.62 (c)	[120] [13 R]
glycerin: see 1,2,3-propanetriol					
glycerol: see 1,2,3-propanetriol					
glycine: see aminoethanoic acid					
glycine, dl-alanyl- : see dl-alanyl-aminoethanoic acid					
glycine, N-benzoyl- : see hippuric acid					
glycine, glycylyl- . (glycylglycine) $H_2NCH_2CONHCH_2COOH$	c c	1941 1964	tc, 87-294 tc, 10-310	45.4 (c)	[112] [123]
glycine, hippuryl- . (hippurylglycine) $C_6H_5CONHCH_2CONHCH_2COOH$	c	1941	tc, 85-297	75.2 (c)	[112]
glycine, dl-leucyl- . (dl-leucylglycine) $(CH_3)_2CHCH_2(NH_2)CHCONHCH_2COOH$	c	1941	tc, 86-297	67.2 (c)	[112]
glycol: see 1,2-ethanediol					
glycolamide: see 2-hydroxyethanamide					
glycolic acid: see ethanoic acid, hydroxy-					
glycyl glycine: see glycine, glycylyl-					
grape sugar: see d-glucose					
guanidine carbonate. $2CH_5N_3 \cdot H_2CO_3$	c	1940	tc, 86-298	70.59 (c)	[116]
guanine. (2-aminohypoxanthine) $C_5H_5N_5O$	c	1935	tc, 84-297	38.3 (c)	[242]
hendecanoic acid: see undecanoic acid					

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298° cal/°K-mol	Reference
heneicosane, 11-n-decyl- $\text{CH}_3(\text{CH}_2)_9\text{CH}(\text{C}_{10}\text{H}_{21})(\text{CH}_2)_9\text{CH}_3$	c, l	1945	tc, 12-298	259.60 (l)	Penn State work [74]
	c, l	1945	tc, 80-297	262.5 (l)	
heptadecanoic acid. (margaric acid) $\text{CH}_3(\text{CH}_2)_{15}\text{COOH}$	c, l	1929	tc-, 291-372		[82]
n-heptaldehyde: see heptanal					
heptanal. (enanthaldehyde), $\text{CH}_3(\text{CH}_2)_5\text{CHO}$	c, l	1956	tc, 80-300	83.3 (l)	[190]
heptane, 4-thia- $\text{C}_3\text{H}_7\text{SC}_3\text{H}_7$	c, l	1961	tc, 13-315	80.85 (l)	[156]
	g	1961		107.16 (g)	[156]
heptanoic acid. (enanthic acid) $\text{CH}_3(\text{CH}_2)_5\text{COOH}$	c, l	1926	tc-, 238-303		[83]
1-heptanol. (n-heptyl alcohol) $\text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{OH}$	c, l	1956	tc, 80-300	77.9 (l)	[190]
1-heptanol, 2-methyl- $\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_3)\text{CH}_2\text{OH}$	gl, l	1931	tc, 102-311		[45]
1-heptanol, 5-methyl- $\text{CH}_3\text{CH}_2(\text{CH}_3)(\text{CH}_2)_5\text{OH}$	gl	1931	tc, 102-299		[45]
2-heptanol, 2-methyl- $(\text{CH}_3)_2\text{COH}(\text{CH}_2)_4\text{CH}_3$	c, l	1931	tc, 102-311		[45]
2-heptanol, 3-methyl- $\text{CH}_3\text{CHOHCH}(\text{CH}_3)(\text{CH}_2)_3\text{CH}_3$	gl	1931	tc, 102-299		[45]
2-heptanol, 4-methyl- $\text{CH}_3\text{CHOHCH}_2\text{CH}(\text{CH}_3)(\text{CH}_2)_2\text{CH}_3$	gl	1931	tc, 102-299		[45]
2-heptanol, 5-methyl- $\text{CH}_3\text{CHOH}(\text{CH}_2)_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$	gl	1931	tc, 102-299		[45]
2-heptanol, 6-methyl- $\text{CH}_3\text{CHOH}(\text{CH}_2)_3\text{CH}(\text{CH}_3)\text{CH}_3$	gl	1931	tc, 102-299		[45]
3-heptanol, 4-methyl- $\text{CH}_3\text{CH}_2\text{CHOHCH}(\text{CH}_3)(\text{CH}_2)_2\text{CH}_3$	gl	1931	tc, 102-299		[45]
3-heptanol, 6-methyl- $\text{CH}_3\text{CH}_2\text{CHOH}(\text{CH}_2)_3(\text{CH}_3)_2$	c, l	1931	tc, 102-323		[45]
4-heptanol, 2-methyl- $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CHOH}(\text{CH}_2)_2\text{CH}_3$	gl	1931	tc, 102-299		[45]
4-heptanol, 4-methyl- $\text{CH}_3(\text{CH}_2)_2\text{COH}(\text{CH}_3)(\text{CH}_2)_2\text{CH}_3$	gl	1931	tc, 102-299		[45]
n-heptoic acid: see heptanoic acid					
n-heptyl alcohol: see 1-heptanol					

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
hexacosanoic acid. (cerotic acid) $\text{CH}_3(\text{CH}_2)_{24}\text{COOH}$	c, l	1929	tc-, 290-382		[82]
hexadecanoic acid. (palmitic acid) $\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$	c c, l c	1925 1926 1929	tc, 88-292 tc-, 295-373	129.9 (c) 113.7 ± 1.14 (c)	[187] [83] [189]
1-hexadecanol. (cetyl alcohol) $\text{CH}_3(\text{CH}_2)_{15}\text{OH}$	c c l	1949 1956 1956	tc, 283-323 tc, 80-290	108.0 (c) 145.0 (l)	[129] [190] [190]
hexadecyl alcohol: see 1-hexadecanol					
hexane, 3,4-dithia- . $(\text{C}_2\text{H}_5\text{S})_2$	c, l g	1952 1958	tc, 13-299 tc, 408-428	72.90 ± 0.15 (l) 99.07 (g) S(g, 373.73) = 107.31 S(g, 400.04) = 109.96	[222] [110]
hexane, 2-thia- . $\text{CH}_3\text{SC}_4\text{H}_9$	c, l g	1961 1961	tc, 12-358	73.49 (l) 98.43 (g)	[156] [156]
hexane, 3-thia- . $\text{C}_2\text{H}_5\text{SC}_3\text{H}_7$	c, l g	1961 1961	tc, 12-366	73.98 (l) 98.82 (g)	[156] [156]
1,2,3,4,5,6-hexanehexol. (dulcitol), $\text{CH}_2\text{OH}(\text{CHOH})_4\text{CH}_2\text{OH}$	soln  c c	1901  1926 1929	tc-, 298 (400-500 moles $\text{H}_2\text{O}$ containing 1 mole dulcitol) tc, 38-293	59.2 (c) 56.0 ± 0.6 (c)	[150] [182] [189]
hexanoic acid. (n-caproic acid) $\text{CH}_3(\text{CH}_2)_4\text{CO}_2\text{H}$	c, l	1926	tc-, 240-296		[33]
hexanoic acid, 6-amino-, lactam. (ε-caprolactam) $\text{C}_6\text{H}_{11}\text{NO}$	c, l c, l	1959 1962	tc, 60-370 tc, 60-375	40.3 (c) 40.3 ± 0.4 (c)	[137] [136]
hexanoic acid, 6-amino-, lactam, polymer. (poly-ε-caprolactam), $(\text{C}_6\text{H}_{11}\text{NO})_x$	c	1962	tc, 63-365	41.4 ± 0.4 (c)	[136]
hexanoic acid, 4-2,6-diamino-, hydrochloride. (l-lysine hydrochloride), $(\text{NH}_3\text{Cl})(\text{CH}_2)_4(\text{NH}_2)\text{CHCOOH}$	c c	1963 1964	tc, 11-305 tc, 0-300 th, 0-300	63.21 (c) 63.127 (c)	[45] [136]
1-hexanol. $\text{CH}_3(\text{CH}_2)_4\text{CH}_2\text{OH}$	c, l	1929	tc, 18-290	68.6 ± 0.4 (l)	[131]
2-hexanone, 1,3,4,5,6-pentahydroxy- . (l-sorbose) $\text{C}_6\text{H}_{12}\text{O}_6$	c	1941	tc, 64-296	52.8 (c)	[126]
n-hexyl alcohol: see 1-hexanol					
hippuric acid. (N-benzoylglycine), $\text{C}_6\text{H}_5\text{CONHCH}_2\text{COOH}$	c	1941	tc, 85-298	57.2 (c)	[112]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
<i>l</i> -histidine hydrochloride. ( <i>l</i> -α-amino-5-imidazole-propanoic acid hydrochloride), $C_3H_3N_2(HCl)CH_2(NH_2)CHCOOH$					
	c	1963	tc, 11-305	65.99 (c)	[48]
	c	1964	tc, 0-300 th, 0-300	65.992 (c)	[13 R]
hydrazine. $NH_2NH_2$					
	c, l	1949	tc, 12-340	28.97 ±0.10 (l)	[229]
	g	1949		56.97 ±0.30 (g)	[229]
hydrazine, sym-dimethyl- . $CH_3NHNHCH_3$					
	c, l	1951	tc, 15-298	47.598±0.12 (l)	[17]
	g	1951		74.39 ±0.2 (g)	[17]
hydrazine, unsym-dimethyl- . $NH_2N(CH_3)_2$					
	c, l	1953	tc, 13-298	47.86 ±0.12 (l)	[20]
	g	1953		72.82 ±0.20 (g)	[20]
hydrazine, methyl- . $CH_3NHNH_2$					
	c, l	1951	tc, 15-298	39.66 ±0.07 (l)	[16]
	g	1951	tc, 298-1500	66.61 ±0.20 (g)	[16]
hydrocyanic acid. (hydrogen cyanide) HCN					
	g	1936	tc, 303-421		[68]
	c, l	1939	tc, 15-298	26.97 ±0.05 (l)	[87]
	g	1939		47.92 (g)	[87]
hydrogen cyanide: see hydrocyanic acid					
hydroquinol: see 1,4-dihydroxybenzene (hydroquinone)					
hydroquinone: see 1,4-dihydroxybenzene					
hydroxylamine hydrochloride. $NH_2OH \cdot HCl$					
	c	1941	tc-, 273-373		[216]
<i>l</i> -hydroxyproline: see proline, <i>l</i> -hydroxy-					
hypoxanthine. (6-oxypurine) $C_5H_4N_4O$					
	c	1935	tc, 85-298	34.8 (c)	[242]
hypoxanthine, 2-amino- : see guanine					
insulin: see zinc-insulin					
isoamyl alcohol: see 3-methyl-1-butanol					
isobutyl alcohol: see 2-methyl-1-propanol					
isoleucine: see d-2-amino-3-methylpentanoic acid					
isophthalic acid: see 1,3-benzenedicarboxylic acid					
isoprene: see 2-methyl-1,3-butadiene					
isopropyl alcohol: see 2-propanol					
isopropyl ether: see propane, 2-isopropoxy-					
lactamide: see 2-hydroxypropanamide					
d( <i>l</i> )-lactic acid: see d( <i>l</i> )-2-hydroxypropanoic acid					
<i>l</i> (d-)-lactic acid: see <i>l</i> (d-)-2-hydroxypropanoic acid					

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
lactic acid, thio- : see 2-mercaptopropanoic acid					
$\alpha$ -lactose. (milk sugar), (4-( $\alpha$ -d-galactosido)-d-glucose), $C_{12}H_{22}O_{11}$	soln	1901	tc-, 298 (200-300 moles H <sub>2</sub> O con- taining 1 mole sugar)		[150]
	soln	1936	tc-, 293 (3-20% aq soln)		[26]
$\alpha$ -lactose monohydrate. (4-( $\alpha$ -d-galactosido)-d-glucose hydrate) $C_{12}H_{22}O_{11} \cdot H_2O$					
	c	1941	tc, 61-297	99.1 (c)	[5]
$\beta$ -lactose. (4-( $\beta$ -d-galactosido)-d-glucose) $C_{12}H_{22}O_{11}$					
	c	1936	tc, 83-298	96.4 (c)	[78]
	c	1941	tc, 66-289	92.3 (c)	[5]
lauric acid: see dodecanoic acid					
dl-leucine: see dl-2-amino-4-methyl-pentanoic acid					
l-leucine: see l-2-amino-4-methyl-pentanoic acid					
dl-leucylglycine: see glycine, dl-leucyl-					
levulose: see d-fructose					
lignoceric acid. $C_{23}H_{47}COOH$					
	c, l	1929	tc-, 291-382		[32]
l-lysine hydrochloride: see d-2,6-diaminohexanoic acid, hydrochloride					
maleic acid: see cis-butenedioic acid					
l-malic acid: see l-hydroxybutanedioic acid					
$\beta$ -maltose monohydrate. (4-( $\alpha$ -d-glucosido)-d-glucose) $C_{12}H_{22}O_{11} \cdot H_2O$					
	c	1941	tc, 61-296	99.8 (c)	[5]
maltose - water mixture. $C_{12}H_{22}O_{11} \cdot H_2O$					
	soln	1901	tc-, 298 (300-445.4 moles H <sub>2</sub> O containing 1 mole sugar)		[150]
mandelic acid: see ethanoic acid, hydroxy-(phenyl)-					
mannite: see mannitol					
d-mannitol. (d-mannite), $CH_2OH(CHOH)_4CH_2OH$					
	c	1865	tc-, 292-325		[139]
	soln	1899	tc-, 298 (100-400 moles H <sub>2</sub> O con- taining 1 mole mannite)		[149]
	soln	1901	tc-, 298 (107.3-500 moles H <sub>2</sub> O con- taining 1 mole mannite)		[150]
	c	1926	tc, 88-294	60.5 (c)	[181]
	c	1929		57.0 $\pm$ 0.6 (c)	[189]
	c, l	1932	tc, 303-473		[239]
	soln	1936	tc, 298 (0.01-0.9995 molal)		[258]
margaric acid: see heptadecanoic acid					

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
methanamide. (formamide), $\text{HCONH}_2$	c l g	1958 1958 1958	tc, 298-1000 (pressure=1 atm)	(21.6) (c) (27.4) (l) (59.38) (g)	[24] [24] [24]
methanamide, dimethyl- . $\text{HCON}(\text{CH}_3)_2$	l, g	1961	tc, 83-323	28.5 (g)	[85]
methane, amino- : see methylamine					
methane, methylsulfinyl- . (methyl sulfoxide), $\text{CH}_3\text{SOCH}_3$	g	1962	tc, 298-1000	73.20	[147]
methane, methylsulfonyl- . (methyl sulfone), $\text{CH}_3\text{SO}_2\text{CH}_3$	g	1962	tc, 298	74.2	[147]
methane, nitro- . $\text{CH}_3\text{NO}_2$	g g c, l	1941 1942 1947	tc, 341-448 tc, 378-434 tc, 13-297	65.64 ± 0.15 (g) [60] 65.73 ± 0.10 (g)	[199] [60] [128]
methane, phenyl- : see methylbenzene					
methanethiol. (methyl mercaptan). $\text{CH}_3\text{SH}$	c, l	1942	tc, 15-271	$S^\circ(l, 279.12) = 39.01$ $S^\circ(g, 279.12) = 60.16 \pm 0.10$	[208]
methanoate, ethyl. $\text{HCOOC}_2\text{H}_5$	g	1938	tc, 410		[27]
methanoic acid. (formic acid), $\text{HCOOH}$	c, l c soln  c, l g soln	1920 1929 1936  1941 1958 1958	tc, 71-292  tc, 298-353 (aq, 16-100% Formic acid by weight) tc, 15-300  tc, 273-393 (0.491-2.84 mol/kg-H <sub>2</sub> O)	34.2 (l) 30.7 ± 0.3 (l)  30.82 ± 0.1 (l) (60.1) (g)	[89] [189] [93] [244] [2] [2]
methanoic acid dimer. $(\text{HCOOH})_2$	g	1959		$S(g, 373) = 18.60 \pm 0.3$	[164]
methanol. $\text{CH}_3\text{OH}$	l c, l c, l c, l l l l c g c, l g  g  c, l c, l	1907 1925 1925 1929 1929 1929 1931 1937 1941 1949 1953  1957  1962 1962	tc-, 276-315 tc, 89-290 th, 89-290 tc, 19-292 tc, 190-265  th, 313-383 tc, 4-28 tc, 350-443 tc, 90-273 tc, 341-405 (pressure = 750 mm) tc, 513-523 (18-60 atm pressure) tc, 5-325 tc, 149-171	32.6 (l) 30.3 ± 0.2 (l) 31.0 ± 0.3 (l) 30.3 (l)  30.40 (l)	[35] [180] [146] [130] [163] [189] [73] [3] [59] [240] [234] [4] [38] [257]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
methanol - water mixture. $\text{CH}_3\text{OH} - \text{H}_2\text{O}$	soln	1907	tc-, 273-315 (0-100% alcohol by weight)		[35]
methanol, diphenyl- . $(\text{C}_6\text{H}_5)_2\text{CHOH}$	c	1931	tc, 102-299		[237]
l-methionine: see l-2-amino-4-methylthio-butanolic acid					
methoxymethane. $\text{CH}_3\text{OCH}_3$	g c, l	1940 1941	tc-, 272-370 tc, 14-245	(44.98 ± 0.40) (l) (63.72 ± 0.20) (g) $S^\circ(l, 200.00)$ = 35.03 ± 0.07 $S^\circ(g, 200.00)$ = 58.03 ± 0.10	[135] [134] [134]
methyl acetate: see methylethanoate					
methyl alcohol: see methanol					
methylamine. (aminomethane), $\text{CH}_3\text{NH}_2$	g c, l l	1933 1937 1939	tc, 273-323 tc, 13-259 tc, 185-260	(35.90) (l) $S^\circ(l, 266.84) = 33.21$	[69] [19] [14]
methyl ether: see methoxymethane					
methyl ethyl ketone: see 2-butanone					
methyl isothiocyanate $\text{CH}_3\text{SCN}$	g	1963	tc, 273.15-1000	69.29 (g)	[148]
methyl nitrate $\text{CH}_3\text{NO}_3$	c, l	1953	tc, 14-296	51.86 (l)	[94]
methyl n-propyl ketone: see 2-pentanone					
methyl sulfone: see methylsulfonylmethane					
methyl sulfoxide: see methylsulfinylmethane					
milk sugar: see α-lactose					
α-monopalmitin: see 1,2,3-propanetriol, monohexadecanoate (β)					
β-monopalmitin: see 1,2,3-propanetriol, monohexadecanoate (α)					
myristic acid: see tetradecanoic acid					
naphthalene, 1,5-dinitro- . $\text{C}_{10}\text{H}_6(\text{NO}_2)_2$	c	1941	tc-, 273-373		[216]
naphthalene, 1,8-dinitro- . $\text{C}_{10}\text{H}_6(\text{NO}_2)_2$	c	1941	tc-, 273-373		[216]
naphthalene, 1-hydroxy- . (α-naphthol), $\text{C}_{10}\text{H}_7\text{OH}$	c, l	1926	th, 293-453		[11]
naphthalene, 2-hydroxy- . (β-naphthol), $\text{C}_{10}\text{H}_7\text{OH}$	c, l	1926	th, 293-478		[11]

<u>Substance</u>	<u>Phase</u>	<u>Year</u>	<u>Temperature Range of Heat Data, °K</u>	<u>Entropy at 298°K cal/°K-mol</u>	<u>Reference</u>
$\alpha$ -naphthol: see 1-hydroxynaphthalene					
$\beta$ -naphthol: see 2-hydroxynaphthalene					
$\beta$ -naphthyl salicylate: see benzoic acid, 2-hydroxy-, 2-naphthyl ester					
nonane, 5-thia- $C_4H_9SC_4H_9$	c, l g	1961 1961	tc, 12-356	96.82 (l) 125.69 (g)	[156] [156]
nonanoic acid. $CH_3(CH_2)_7COOH$	c, l c	1924 1926	tc-, 257-317 tc-, 231-289		[84] [83]
nonoic acid: see nonanoic acid					
octadecanoic acid. (stearic acid), $CH_3(CH_2)_{16}COOH$	l	1930	tc-, 366-526		[142]
cis-9-octadecenoic acid. (oleic acid), $C_8H_{17}CH=CH(CH_2)_7COOH$	l	1930	tc-, 283-430		[142]
octane, 4,5-dithia- $(C_3H_7S)_2$	c, l	1958	tc, 12-351	89.28 (l) 118.30 (g)	[110]
octanoic acid. (caprylic acid), $CH_3(CH_2)_6COOH$	c, l	1924	tc-, 273-319		[84]
1-octanol. $CH_3(CH_2)_6CH_2OH$	c, l	1931	tc, 102-286		[45]
2-octanol. $CH_3CHOH(CH_2)_5CH_3$	c, l	1931	tc, 102-299		[45]
3-octanol. $CH_3CH_2CHOH(CH_2)_4CH_3$	c, l	1931	tc, 102-299		[45]
4-octanol. $CH_3(CH_2)_2CHOH(CH_2)_3CH_3$	c, l	1931	tc, 102-311		[45]
n-octoic acid: see octanoic acid					
oleic acid: see cis-9-octadecenoic acid					
dl-ornithine: see dl-2,5-diaminopentanoic acid					
ornithine dihydrochloride: see 2,5-diaminopentanoic acid dihydrochloride					
oxalic acid: see ethanedioic acid					
palm oil	l	1944	tc-, 318-323		[104]
palm oil stearine.	c, l	1944	tc-, 273-373		[104]
palmitic acid: see hexadecanoic acid					
pentacosanic acid: see pentacosanoic acid					
pentacosanoic. $C_{24}H_{49}COOH$	c, l	1929	tc-, 293-383		[82]



Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
pentadecanoic acid. (pentadecic acid), $\text{CH}_3(\text{CH}_2)_{13}\text{COOH}$	c, l	1926	tc-, 293-361		[83]
pentadecic acid: see pentadecanoic acid					
pentane, 2-thia- . $\text{CH}_3\text{SC}_3\text{H}_7$	c, l	1957	tc, 13-326	65.14 (l)	[224]
pentane, 3-thia- . $(\text{C}_2\text{H}_5)_2\text{S}$	c, l g	1952 1959	tc, 16-316	64.36 $\pm$ 0.10 (l) 87.96 (g)	[221] [226]
pentanedioic acid, d-2-amino- . (l-glutamic acid), $\text{HOOC}(\text{CH}_2)_2(\text{NH}_2)\text{CHCOOH}$	c	1944	tc, 102-301	45.2 (c)	[175]
	c	1963	tc, 9-303	44.98 (c)	[120]
	c	1964	tc, 0-300 th, 0-300	44.982 (c)	[13 R]
pentanedioic acid, d-2-amino- , $\gamma$ -benzyl- , polymer. (poly- $\gamma$ -benzyl-l-glutamate) $(\text{HOOC}(\text{CH}_2)_2\text{CH}(\text{NH}_2)\text{COOCH}_2\text{C}_6\text{H}_5)_x$ soln		1964	tc, 283-326 (0.257 mol/kg-solvent) solvent = dichloroacetic acid and 1,2-dichloroethane		[1]
pentanedioic acid, l-2-amino- . (d-glutamic acid), $\text{HOOC}(\text{CH}_2)_2\text{CH}(\text{NH}_2)\text{COOH}$	c	1932	tc, 91-295	45.7 (c)	[113]
pentanedioic acid, l-2-amino- , hydrochloride. (d-glutamic acid hydrochloride), $\text{HOOC}(\text{CH}_2)_2(\text{NH}_3\text{Cl})\text{CHCOOH}$	c	1940	tc, 85-297	59.33 (c)	[116]
1-pentanethiol. (amyl mercaptan), $\text{CH}_3(\text{CH}_2)_4\text{SH}$	c, l	1952	tc, 13-321	74.18 $\pm$ 0.15 (l) 99.18 $\pm$ 0.35 (g)	[72]
pentanoic acid, d-2-amino-3-methyl- . (l-isoleucine), $(\text{CH}_3)(\text{C}_2\text{H}_5)\text{CH}(\text{NH}_2)\text{CHCOOH}$	c c	1963 1964	tc, 11-306 tc, 0-300 th, 0-300	49.71 (c) 49.632 (c)	[122] [13 R]
pentanoic acid, dl-2-amino-4-methyl- . (dl-leucine) $(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{NH}_2)\text{COOH}$	c	1937	tc, 86-297	49.5 (c)	[115]
pentanoic acid, l-2-amino-5-guanido- . (d-arginine) $\text{NH}_2\text{C}(=\text{NH})\text{NH}(\text{CH}_2)_3(\text{NH}_2)\text{CHCOOH}$	c	1937	tc, 86-297	59.9 (c)	[115]
pentanoic acid, l-2-amino-4-methyl- . (l-leucine) $(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{NH}_2)\text{CHCOOH}$	c c	1963 1964	tc, 11-305 tc, 0-300 th, 0-300	50.62 (c) 50.598 (c)	[122] [13 R]
pentanoic acid, 5-amino- , lactam. (2-piperidone) $\text{NHCOCH}_2\text{CH}_2\text{CH}_2\text{CH}_2$	c, l c, l	1959 1962	tc, 60-350 tc, 61-350	39.4 (c) 39.4 $\pm$ 0.4 (c)	[137] [136]
pentanoic acid, 5-amino- , lactam, polymer. (polypiperidone) $(\text{NHCO}(\text{CH}_2)_4)_x$	c	1962		33.4 $\pm$ 1.1 (c)	[136]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
pentanoic acid, dl-2,5-diamino- . (dl-ornithine), $\text{NH}_2(\text{CH}_2)_3(\text{NH}_2)\text{CHCOOH}$	c	1940	tc, 89-298	46.2 (c)	[118]
pentanoic acid dihydrochloride, 2,5-diamino- . (ornithine dihydrochloride) $(\text{NH}_3\text{Cl})(\text{CH}_2)_3(\text{NH}_3\text{Cl})\text{CHCOOH}$	c	1940	tc, 85-293	70.25 (c)	[116]
pentanoic acid hydrochloride, d-2-amino-5-guanido- . (l-arginine hydrochloride), $\text{NH}_2\text{C}(=\text{NH}_2\text{Cl})\text{NH}(\text{CH}_2)_3(\text{NH}_2)\text{CHCOOH}$	c	1963	tc, 11-304	68.43 (c)	[48]
	c	1964	tc, 0-300		
			th, 0-300	68.404 (c)	[13 R]
1-pentanol. (n-amyl alcohol), $\text{CH}_3(\text{CH}_2)_3\text{CH}_2\text{OH}$	l	1907	tc-, 224-264		[22]
	c, l	1933	tc, 94-298	60.9 (l)	[185]
	l	1949	tc, 313-343		[143]
	g	1953	tc, 417-437 (pressure 750 mm)		[234]
3-pentanol. (diethylcarbinol), $\text{CH}_3\text{CH}_2\text{CHOHCH}_2\text{CH}_3$	l	1949	tc, 313-343		[143]
2-pentanone. $\text{CH}_3\text{COCH}_2\text{CH}_2\text{CH}_3$	g	1961	tc, 369-454	91.61 (g)	[172]
phenol. $\text{C}_6\text{H}_5\text{OH}$	soln	1901	tc-, 298 (300 moles $\text{H}_2\text{O}$ containing 1 mole phenol)		[150]
	c	1925	th, 89-290		[146]
	c	1933	tc, 93-296	34.1 (c)	[185]
	l	1933		42.6 (l)	[185]
	c	1935	tc, 78-229		[12]
	l	1959	tc, 363-388		[145]
	c, l	1963	tc, 13-336	34.420 (c)	[7]
phenol, 2-acetamino- : see ethanamide, N(2-hydroxyphenyl)-					
phenol, 3-acetamino- : see ethanamide, N(3-hydroxyphenyl)-					
phenol, 4-acetamino- : see ethanamide, N(4-hydroxyphenyl)-					
phenol, 2-nitro- . $\text{NO}_2\text{C}_6\text{H}_4\text{OH}$	l	1959	tc, 363-408		[145]
phenol, 3-nitro- . $\text{NO}_2\text{C}_6\text{H}_4\text{OH}$	l	1959	tc, 388-408		[145]
phenol, 4-nitro- . $\text{NO}_2\text{C}_6\text{H}_4\text{OH}$	l	1959	tc, 388-408		[145]
phenol, thio- : see benzenethiol					
phenol, 2,4,6-trinitro- . (picric acid), $(\text{NO}_2)_3\text{C}_6\text{H}_2\text{OH}$	c	1924	tc-, 90-395		[249]
phenoxybenzene. (diphenyl ether) $(\text{C}_6\text{H}_5)_2\text{O}$	c	1931	tc, 102-299		[238]
	c, l	1951	tc, 2-570	55.91 (c)	[79]
	c, l	1953	tc, 14-573		[92]
l-phenylalanine: see l-2-amino-3-phenylpropanoic acid					

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
phenyl ether: see phenoxybenzene					
phenyl ketone: see benzophenone					
phosphine, triphenyl- $(C_6H_5)_3P$	c	1931	tc, 102-299		[238]
phosphoric acid, ortho- $H_3PO_4$	soln	1933	tc, 293-373 (0-89.72% $H_3PO_4$ )		[200]
	soln	1933	tc, 292-373 (0-89.72% $H_3PO_4$ )		[202]
	c	1956	tc, 15-370		[81]
	c	1957	tc, 10-300	26.41 (c)	[64]
	soln	1958	tc, 288-353 (4.46-84.81% aq $H_3PO_4$ )		[63]
phosphoric acid, ortho-, hemihydrate. $2H_3PO_4 \cdot H_2O$	c	1957	tc, 10-300	61.73 (c)	[64]
phosphorus nitride. $P_3N_5$		1939	tc-, 273-578		[209]
phosphorus pentoxide. $P_2O_5$	c	1963	tc, 12-324.5	54.68 ± 0.1 (c)	[9]
phthalic acid: see 1,2-benzenedicarboxylic acid					
2-phthalic acid: see phthalic acid					
3-phthalic acid: see 1,3-benzenedicarboxylic acid					
4-phthalic acid: see 1,4-benzenedicarboxylic acid					
phthalic anhydride: see 1,2-benzenedicarboxylic acid, anhydride					
picric acid: see 2,4,6-trinitrophenol					
2-piperidone: see 5-aminopentanoic acid lactam					
polypiperidone: see poly-5-aminopentanoic acid lactam					
polypyrrolidone: see pyrrolidinone, polymer					
potato starch.	suspension	1942	th, 273-313 (18.0-100% starch)		[76]
<i>l</i> -proline. <i>l</i> -2-pyrrolidinecarboxylic acid), $C_4H_8NCOOH$	c	1940	tc, 88-300	40.8 (c)	[118]
	c	1963	tc, 11-302	39.21 (c)	[47]
	c	1964	tc, 0-300 th, 0-300	39.210 (c)	[13 R]
proline, <i>l</i> -hydroxy- $C_4H_7N(OH)COOH$	c	1964	tc, 10-305		[123]
propanamide, 2-hydroxy- (lactamide), $CH_3CH(OH)CONH_2$	soln	1942	tc, 278-313 (0.2-505 molarity)		[98]
propane, 2-isopropoxy- (isopropyl ether), $(CH_3)_2CHOCH(CH_3)_2$	c, l	1933	tc, 92-293	70.4 (l)	[185]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
propane, thia- . (dimethyl sulfide), $(CH_3)_2S$	g c, l	1940 1942	tc, 14-287	$S(g, 291.06) = 69.35$ $(46.94 \pm 0.07) (l)$ $(68.28 \pm 0.10) (g)$ $S^o(l, 291.06) = 46.26$ $S^o(g, 291.06) = 67.87 \pm 0.1$	[178] [179] [179] [179] [179]
1,2-propanediol. (propylene glycol), $CH_2OHCHOHCH_3$	gl, l	1927	tc, 91-277		[183]
propanenitrile. $CH_3CH_2CN$	c, l g	1962 1962	tc, 15-297	$45.25 \pm 0.08 (l)$ $68.75 \pm 0.15 (g)$	[256] [256]
1-propanethiol. (n-propyl mercaptan), $CH_3CH_2CH_2SH$	c, l	1956	tc, 13-315	$57.96 (l)$	[198]
1-propanethiol, 2-methyl- . (isobutyl mercaptan), $(CH_3)_2CHCH_2SH$	c, l	1958	tc, 12-349	$63.66 (l)$	[228]
2-propanethiol. (isopropyl mercaptan), $CH_3CHSHCH_3$	c, l	1954	tc, 13-322	$55.82 (l)$	[158]
2-propanethiol, 2-methyl- . (tert-butyl mercaptan), $(CH_3)_3CSH$	c, l g	1953 1959	tc, 12-329	$58.90 \pm 0.15 (l)$ $80.79 (g)$ $80.78 (g)$	[161] [161] [226]
1,2,3-propanetricarboxylic acid, 2-hydroxy-, monohydrate. (citric acid monohydrate) $(COOH)CH_2C(OH)(COOH)CH_2COOH \cdot H_2O$ c <sup>2</sup>		1962	tc, 22-303	$67.74 \pm 0.14 (c)$	[66]
1,2,3-propanetriol. (glycerol), $CH_2OHCHOHCH_2OH$	soln gl, l gl, l c l gl gl, l l soln gl gl c l gl	1899 1922 1923 1923 1925 1926 1927 1929 1936 1937 1937 1937 1962 1965	tc-, 298 (40.4-500 moles H <sub>2</sub> O con- taining 1 mole glycerine) tc, 19-294 tc, 70-299 tc, 70-280 tc, 11- 13 tc, 70-299 tc, 293 (1.26-11.25% aq soln) tc, 2- 95 th, 167-193 tc, 3- 87 tc, 283-453 tc, 1.5-4.2	$53.2 (l)$ $49.7 \pm .5 (l)$ $48.87 (l)$	[149] [232] [88] [88] [187] [233] [183] [189] [26] [3] [173] [3] [176] [53]
1,2,3-propanetriol— aniline mixture. $C_3H_8O_3-C_6H_5NH_2$	soln	1899	tc-, 298 (12.5-100 moles aniline containing 1 mole glycerine)		[149]
1,2,3-propanetriol—ethanol. $C_3H_8O_3-C_2H_5OH$	soln	1899	tc-, 298 (35.32-141.3 moles alcohol containing 1 mole glycerine)		[149]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
$\beta$ -1,2,3-propanetriol, monohexadecanoate. ( $\alpha$ -monopalmitin), $\text{HOCH}_2\text{CHOHCH}_2\text{OOC}(\text{CH}_2)_{14}\text{CH}_3$	c	1940	tc, 298		[44]
$\alpha$ -1,2,3-propanetriol, monohexadecanoate. ( $\beta$ -monopalmitin) $\text{HOCH}_2\text{CHOHCH}_2\text{OOC}(\text{CH}_2)_{14}\text{CH}_3$	c	1940	tc, 298		[44]
1,2,3-propanetriol, tridodecanoate. (trilaurin) $\text{CH}_3(\text{CH}_2)_{10}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{10}\text{CH}_3]_2$		1947	tc, 330-371		[42]
1,2,3-propanetriol, $\beta$ -tridodecanoate. ( $\beta$ -trilaurin), $\text{CH}_3(\text{CH}_2)_{10}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{10}\text{CH}_3]_2$		1947	tc, 90-257	265.1 (c)	[42]
1,2,3-propanetriol, trihexadecanoate. (tripalmitin) $\text{CH}_3(\text{CH}_2)_{14}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{14}\text{CH}_3]_2$		1947	tc, 338-369		[42]
1,2,3-propanetriol, $\alpha$ -trihexadecanoate. ( $\alpha$ -tripalmitin), $\text{CH}_3(\text{CH}_2)_{14}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{14}\text{CH}_3]_2$	c	1947	tc, 194-252		[42]
1,2,3-propanetriol, $\beta$ -trihexadecanoate. ( $\beta$ -tripalmitin), $\text{CH}_3(\text{CH}_2)_{14}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{14}\text{CH}_3]_2$	c	1947	tc, 87-282	331.6 (c)	[42]
1,2,3-propanetriol, trioctadecanoate. (tristearin) $\text{CH}_3(\text{CH}_2)_{16}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{16}\text{CH}_3]_2$		1947	tc, 346-372		[42]
1,2,3-propanetriol, $\alpha$ -trioctadecanoate. ( $\alpha$ -tristearin) $\text{CH}_3(\text{CH}_2)_{16}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{16}\text{CH}_3]_2$	c	1947	tc, 192-267		[42]
1,2,3-propanetriol, $\beta$ -trioctadecanoate. ( $\beta$ -tristearin) $\text{CH}_3(\text{CH}_2)_{16}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{16}\text{CH}_3]_2$	c	1947	tc, 95-272	366.8 (c)	[42]
1,2,3-propanetriol, tritetradecanoate. (trimyristin) $\text{CH}_3(\text{CH}_2)_{12}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{12}\text{CH}_3]_2$		1947	tc, 331-365		[42]
1,2,3-propanetriol, $\alpha$ -tritetradecanoate. ( $\alpha$ -trimyristin), $\text{CH}_3(\text{CH}_2)_{12}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{12}\text{CH}_3]_2$	c	1947	tc, 192-247		[42]
1,2,3-propanetriol, $\beta$ -tritetradecanoate. ( $\beta$ -trimyristin), $\text{CH}_3(\text{CH}_2)_{12}\text{COOCH}[\text{CH}_2\text{OOC}(\text{CH}_2)_{12}\text{CH}_3]_2$	c	1947	tc, 89-262	297.8 (c)	[42]
1,2,3-propanetriol—glucose mixture. $\text{C}_3\text{H}_8\text{O}_3\text{—C}_6\text{H}_{12}\text{O}_6$	gl, l	1930	tc, 99-284 (50% of each component by weight)		[194] [194]
1,2,3-propanetriol—1,2-propanediol—glucose mixture. $\text{C}_3\text{H}_8\text{O}_3\text{—C}_3\text{H}_8\text{O}_2\text{—C}_6\text{H}_{12}\text{O}_6$	gl, l	1930	tc, 93-281 (33 1/3% of each compo- nent by weight)		[194]
propanoic acid. (propionic acid), $\text{CH}_3\text{CH}_2\text{COOH}$	c soln	1909 1958	tc, 227-253 tc, 273-393 (0.501-2.001 mol/kg- $\text{H}_2\text{O}$ )		[151] [2]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
propanoic acid, 2-amino-, 1-3,3'-dithiobis- . (l-cystine), $(\text{HOOC}(\text{NH}_2)\text{CHCH}_2\text{S-})_2$	c	1935	tc, 86-297	68.5 (c)	[114]
	c	1964	tc, 11-303	67.06 (c)	[124]
	c	1964	tc, 0-300 th, 0-300	67.053 (c)	[13 R]
propanoic acid, d-2-amino- . (l-alanine), $\text{CH}_3(\text{NH}_2)\text{CHCOOH}$	c	1960	tc, 12-305	30.88 (c)	[121]
	c	1964	tc, 0-300 th, 0-300	30.883 (c)	[13 R]
propanoic acid, d-2-amino- and hydrochloric acid aqueous mixture. $\text{CH}_3(\text{NH}_2)\text{CHCOOH-HCl-H}_2\text{O}$	soln	1942	tc, 298 (HCl, 0.2006 to 0.2056 (molality)) (alanine, 0 to 0.06302 (molality))		[246]
propanoic acid, d-2-amino- and sodium hydroxide aqueous mixture. $\text{CH}_3(\text{NH}_2)\text{CHCOOH-NaOH-H}_2\text{O}$	soln	1942	tc, 298 (NaOH, 0.00439 to 0.8676 (molality)) (alanine, 0 to 0.03293 (molality))		[246]
propanoic acid, dl-2-amino- . (dl-alanine), $\text{CH}_3\text{CH}(\text{NH}_2)\text{COOH}$	soln	1935	tc, 298 (0-1.88 molal)		[264]
	c	1937	tc, 85-298	31.6 (c)	[115]
	soln	1942	tc, 278-313 (0.1-1.59 molarity)		[98]
propanoic acid, l-2-amino- . (d-alanine), $\text{CH}_3\text{CH}(\text{NH}_2)\text{COOH}$	c	1932	tc, 84-297	31.6 (c)	[113]
propanoic acid, l-2-amino-3-hydroxy- . (l-serine), $\text{HOCH}_2\text{CH}(\text{NH}_2)\text{COOH}$	c	1964	tc, 11-302	35.65 (c)	[125]
propanoic acid, l-2-amino-3(4-hydroxyphenyl)- . (l-tyrosine) $\text{HOC}_6\text{H}_4\text{CH}_2(\text{NH}_2)\text{CHCOOH}$	c	1937	tc, 87-295	53.0 (c)	[115]
	c	1963	tc, 11-302	51.15 (c)	[47]
	c	1964	tc, 0-300 th, 0-300	51.096 (c)	[13 R]
propanoic acid, l-2-amino-5-imidazole-, hydrochloride: see l-histidine hydrochloride					
propanoic acid, l-2-amino-3-indole- : see l-tryptophan					
propanoic acid, l-2-amino-3-mercapto- . (l-cysteine), $\text{HSCH}_2\text{CH}(\text{NH}_2)\text{COOH}$	c	1935	tc, 85-298	40.6 (c)	[114]
propanoic acid, l-2-amino-3-phenyl- . (l-phenylalanine), $\text{C}_6\text{H}_5\text{CH}_2(\text{NH}_2)\text{CHCOOH}$	c	1963	tc, 11-305	51.06 (c)	[47]
	c	1964	tc, 0-300 th, 0-300	51.005 (c)	[13 R]
propanoic acid, 3-amino- . (β-alanine), $\text{NH}_2\text{CH}_2\text{CH}_2\text{COOH}$	soln	1942	tc, 273-313 (0.1-5.35 molarity)		[98]
propanoic acid, ethyl ester. $\text{CH}_3\text{CH}_2\text{COOC}_2\text{H}_5$	g	1938	tc, 410		[27]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298° cal/°K-mol	Reference
propanoic acid, d(l+)-2-hydroxy- . (d(l+)-lactic acid), $\text{CH}_3\text{CHOHCOOH}$	gl, l c, l	1936 1936	tc, 96-303 tc, (90-300) (Estimated from data on glass and partially crystalline material)		[195]
	c	1940	tc, 84-293	34.30 (c)	[195] [116]
propanoic acid, l(d-)-2-Hydroxy- . (l(d-)-lactic acid), $\text{CH}_3\text{CHOHCOOH}$	c	1940	tc, 84-298	34.00 (c)	[116]
propanoic acid, d-2-hydroxy-, amide: see 2-hydroxypropanamide					
propanoic acid, β-2-mercapto- . (β-thiolactic acid), $\text{CH}_3\text{CHSHCOOH}$	c, l	1935	tc, 85-310	54.7 (l)	[114]
1-propanol. $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$	l gl gl, l c, l gl, l gl, l l l g l g g	1907 1913 1920 1926 1927 1927 1929 1929 1938 1941 1953 1961	tc-, 276-317 tc-, 20- 80 tc, 77-275 tc, 88-275 tc, 86-275 tc, 86-275 tc, 163-274 tc, 410 tc, 278-319 tc, 373-437 (pressure 750 mm) tc, 371-452 (1/3 to 5/3 atm)	51.2 (l) 46.1 ± 0.5 (l) 77.63 (g)	[35] [61] [90] [182] [182] [183] [163] [189] [27] [263] [234] [152]
1-propanol-water mixture. $\text{C}_3\text{H}_7\text{OH}-\text{H}_2\text{O}$	soln	1907	tc-, 273-315 (0-100% alcohol by weight)		[35]
1-propanol, 2-methyl. $(\text{CH}_3)_2\text{CHCH}_2\text{OH}$	l g l g l l	1924 1938 1941 1953 1958 1958	tc, 303-344 tc, 410 tc, 277-319 tc, 383-437 (pressure 750 mm) tc-, 295-379 tc-, 295-379		[259] [27] [263] [234] [247] [248]
2-propanol. $\text{CH}_3\text{CHOHCH}_3$	l c, l c, l c, l l g g l l g l c, l g g g	1924 1925 1928 1929 1929 1938 1940 1948 1953 1958 1958 1963 1963 1963 1964	tc, 303-326 tc, 71-293 tc, 71-293 tc, 19-293 tc, 410 tc, 428-480 th, 273-473 tc, 359-437 (pressure 750 mm) tc-, 294-354 tc-, 294-354 tc, 12-327 tc, 359-473 (0.25-1.0 atm pressure) tc, 273.15-1000 tc, 371-452 (1/3 - 4/3 atm)	45.6 (l) 46.1 (l) 43.0 ± 0.3 (l) 43.1 ± 0.4 (l) 74.07 (g)	[259] [187] [188] [132] [189] [27] [192] [91] [234] [247] [248] [8] [106] [97] [29]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298° cal/°K-mol	Reference
2-propanol, 2-methyl- $(\text{CH}_3)_2\text{CHOH}$	c, l	1903	th, 251-318		[58]
	c, l	1926	tc, 87-300	47.2 (l)	[181]
	l	1929		45.3 ± 0.5 (l)	[189]
	g	1950	tc, 411-433 (760 mm pressure)		[204]
	g	1953	tc, 359-437 (750 mm pressure)		[234]
	c, l	1963	tc, 15-331	40.84 (c)	[174]
	g	1963	tc, 363-437 (pressure 1/3-4/3 atm)	77.98 (g)	[31]
2-propanone. (acetone), $\text{CH}_3\text{COCH}_3$	c, l	1925	th, 89-290		[146]
	c, l	1925	tc, 70-289	52.0 (l)	[187]
	c, l	1928	tc, 70-289	52.7 (l)	[188]
	c, l	1929	tc, 18-297	47.9 ± 0.3 (l)	[132]
	l	1929	tc, 205-256		[163]
	l	1929		47.8 ± 0.5 (l)	[189]
	g	1938	tc, 410		[27]
	g	1949	tc, 333-438		[50]
	l	1962	tc, 253-308		[144]
propionic acid: see propanoic acid					
propionitrile: see propanenitrile					
n-propyl alcohol: see 1-propanol					
propylene glycol: see 1,2-propanediol					
purine, 2-amino-, 6-hydroxy- : see guanine					
purine, 6-amino- . (adenine), $\text{C}_5\text{H}_4\text{N}_4\text{NH}_2$	c	1935	tc, 88-298	36.1 (c)	[242]
purine, 2-6-dioxy- : see xanthine					
purine, 6-oxy- : see hypoxanthine					
purine, 2,6,8-trihydroxy- . (uric acid), $\text{C}_5\text{H}_4\text{N}_4\text{O}_3$	c	1935	tc, 86-297	41.4 (c)	[242]
pyridine: see azine					
pyrocatechin: see 1,2-dihydroxybenzene (pyrocatechol)					
pyrocatechol: see 1,2-dihydroxybenzene					
pyrotartaric acid: see methylbutanedioic acid					
pyrrole: see azole					
pyrrolidine. (tetrahydropyrrole), $\text{NHCH}_2\text{CH}_2\text{CH}_2\text{CH}_2$	c, l	1959	tc, 13-351	48.76 (l)	[153]
	c, l	1959	tc, 14-312	48.78 ± 0.10 (l)	[109]
	g	1959	tc, 298-1000	74.00 ± 0.20 (g)	[109]
pyrrolidine, 2-oxo- : see 2-pyrrolidone					
l-2-pyrrolidinecarboxylic acid: see l-proline					
pyrrolidinone, polymer. (poly-2-oxopyrrolidine), $(\text{NHCO}(\text{CH}_2)_3)_x$	c	1962		25.4 ± 1.4 (c)	[136]
2-pyrrolidone. $\text{NHCOCH}_2\text{CH}_2\text{CH}_2$	c, l	1959	tc, 60-335	32.7 (c)	[137]
	c, l	1962	tc, 60-350	32.7 ± 0.4 (c)	[136]



<u>Substance</u>	<u>Phase</u>	<u>Year</u>	<u>Temperature Range of Heat Data, °K</u>	<u>Entropy at 298°K cal/°K-mol</u>	<u>Reference</u>
quinhydrone, (benzoquinhydrone), $C_6H_4O_2 \cdot C_6H_4(OH)_2$	c	1924	tc, 20-243		[141]
quinol: see 1,4-dihydroxybenzene					
CO in $\beta$ -quinol clathrate. (CO in 1,4-benzenediol clathrate), CO in $C_6H_4(OH)_2$		1963	tc, 15-100		[52]
$\beta$ -quinol clathrates of CO. $xCO \cdot 3C_6H_4(OH)_2$ ( $x = 0.4-0.8$ )		1963	tc, 13-300 ( $y = 0.4-0.8$ )	20.94	[241]
$N_2$ in $\beta$ -quinol clathrate. ( $N_2$ in 1,4-benzenediol clathrate), $N_2$ in $C_6H_4(OH)_2$		1963	tc, 15-100		[52]
quinoline: see 1-benzazine					
para-quinone: see 1,4-benzoquinone					
racemic acid; see dl-2,3-dihydroxybutanedioic acid					
resorcin: see resorcinol					
resorcinol: see 1,3-dihydroxybenzene					
saccharose: see sucrose					
salicylic acid: see 2-hydroxybenzoic acid					
semicarbazide hydrochloride. $NH_2CONHNH_2 \cdot HCl$	c	1941	tc-, 273-373		[216]
l-serine: see l-2-amino-3-hydroxy-propanoic acid					
serum albumin, bovine, anhydrous.	c	1964	tc, 10-310		[119]
serum albumin, bovine, hydrated.	c	1964	tc, 10-310		[119]
sesame oil.	l	1944	tc-, 368-373		[104]
l-sorbose: see 1,3,4,5,6-pentahydroxy-2-hexanone					
stearic acid: see octadecanoic acid					
succinamic acid: see butanedioic acid, monoamide					
succinamide: see butanedioic acid, diamide					
succinic acid: see butanedioic acid					
succinimide: see butanedioic acid, imide					
succinonitrile: see butanedinitrile					
sucrose. (( $\alpha$ -d-glucosido)- $\beta$ -d-fructofuranoside), $C_{12}H_{22}O_{11}$	c	1865	tc-, 293-325		[139]
	c	1929	tc-, 293-356		[262]
	c	1933	tc, 94-297	86.1 (c)	[185]
	c	1950	tc, 276-300		[6]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
sucrose-water mixture. $C_{12}H_{22}O_{11} \cdot H_2O$	soln	1899	tc-, 298 (50-250 moles $H_2O$ con- taining 1 mole sugar)		[149]
	soln	1928	tc-, 294-354 (10-75% sucrose)		[261]
	soln	1929	tc-, 294-354 (14.5-81.8% sucrose)		[262]
	soln	1935	tc, 275-312 (0.1-1.0 gm-mole/kg- $H_2O$ )		[77]
	soln	1936	tc, 293 (5-16% aq soln)		[26]
	soln	1937	tc, 293-298 (0.1-2.58 molarity)		[99]
sugar beet (slices).	c	1952	tc-, 293-380		[217]
sulfanilamide: see 4-amino-benzenesulfonic acid, amide					
sunflower stearine.	c, l	1944	tc-, 273-373		[104]
dl-tartaric acid: see dl-2,3-dihydroxybutanedioic acid					
d-tartaric acid: see d-2,3-dihydroxybutanedioic acid					
meso-tartaric acid: see meso-2,3-dihydroxybutanedioic acid					
taurine. (2-aminoethanesulfonic acid), $(NH_2)(CH_2)_2SO_3H$	c	1940	tc, 87-300	36.8 (c)	[118]
terephthalic acid: see 1,4-benzenedicarboxylic acid					
tetradecanoic acid. (myristic acid), $CH_3(CH_2)_{12}COOH$	c, l	1926	tc-, 296-357		[83]
tetryl. (N-methyl-N-2,4,6-tetranitroaniline), $(NO_2)_3C_6H_2N(NO_2)CH_3$	c	1924	tc-, 90-370		[249]
tetryl-2,4,6-trinitrophenol mixture $C_7H_5N_5O_8 \cdot C_6H_3N_3O_7$	c	1924	tc-, 90-353		[249]
tetryl-2-trinitrotoluene mixture. $C_7H_5N_5O_8 \cdot C_7H_5N_3O_6$	c	1924	tc-, 90-333		[249]
thiofuran: see thiophene					
thionaphthene: see 2,3-benzothiophene					
thiophene. $SCH=CHCH=CH$	l	1934	tc, 238-289	42.2 $\pm$ 1.0 (l)	[127]
	c, l	1949	tc, 12-336	43.30 $\pm$ 0.10 (l)	[253]
	g	1957	tc, 300-1000	(S(g, 318.5) = 68.73)	[33]
thiophene, 2,3-benzo- . $C_6H_4SCHCH$	c, l	1954	tc, 12-330	42.329 $\pm$ 0.12 (l)	[71]
thiophene, 2,5-dimethyl- . (2,5-thioxene), $(CH_3)_2C_4H_2S$	c, l	1962	tc, 5-304	58.494 (l) Stable Phase 58.716 (l)	[38]
	c, l	1965	tc, 5-236	58.49 (l) Stable Phase 58.7 (l) Metastable Phase	
					[39]

<u>Substance</u>	<u>Phase</u>	<u>Year</u>	<u>Temperature Range of Heat Data, °K</u>	<u>Entropy at 298°K cal/°K-mol</u>	<u>Reference</u>
thiophene, 2-methyl- . ( $\alpha$ -thiotolene), $\text{CH}_3\text{C}_4\text{H}_3\text{S}$	c, l c c	1956 1962 1962	tc, 12-344 tc, 100-200 tc, 110-200	52.22 (l)	[197] [257] [38]
thiophene, 3-methyl- . ( $\beta$ -thiotolene), $\text{CH}_3\text{C}_4\text{H}_3\text{S}$	c, l g	1953 1959	tc, 12-337	52.185 $\pm$ 0.10 (l) 76.84 (g)	[162] [226]
thiourea: see urea, 2-thio-					
l-threonine: see l-2-amino-3-hydroxy-butanoic acid					
toluene: see methylbenzene					
toluene, 2-amino-5-nitro- . $\text{NO}_2\text{C}_6\text{H}_3(\text{CH}_3)\text{NH}_2$	c	1941	tc-, 273-373		[215]
toluene, 4-amino-3-nitro- . $\text{NO}_2\text{C}_6\text{H}_3(\text{CH}_3)\text{NH}_2$	c	1941	tc-, 273-373		[215]
toluene, trinitro- . $(\text{NO}_2)_3\text{C}_6\text{H}_2\text{CH}_3$	c	1924	tc-, 90-352		[249]
toluhydroquinone: see 2-methyl-1,4-dihydroxybenzene					
ortho-toluic acid: see 2-methylbenzoic acid					
meta-toluic acid: see 3-methylbenzoic acid					
para-toluic acid: see 4-methylbenzoic acid					
toluidine, nitro-(1,2,5): see 2-amino-5-nitrotoluene					
toluidine, nitro-(1,4,3): see 4-amino-3-nitrotoluene					
tricosanic acid: see tricosanoic acid					
tricosanoic acid $\text{C}_{22}\text{H}_{45}\text{COOH}$	c, l	1929	tc-, 291-382		[82]
tridecanoic acid. (n-tridecoic acid), $\text{CH}_3(\text{CH}_2)_{11}\text{COOH}$	c, l	1926	tc-, 273-349		[83]
tridecoic acid: see tridecanoic acid					
triethylenediamine. (1,4-diazabicyclo [2,2,2] octane), $\text{C}_6\text{H}_{12}\text{N}_2$	c c, l	1960 1963	tc, 5-344 tc, 300-450	37.67 37.67	[40] [251]
trilaurin: see 1,2,3-propanetriol, tridodecanoate					
trimethylamine $(\text{CH}_3)_3\text{N}$	c, l	1944	tc, 12-276	(49.82) (l) $S^\circ(1,276.03)$ $= 47.28 \pm 0.14$	[18]
trimyristin: see 1,2,3-propanetriol, tritetradecanoate					
tripalmitin: see 1,2,3-propanetriol, trihexadecanoate					
triphenylamine $(\text{C}_6\text{H}_5)_3\text{N}$	c	1931	tc, 102-346		[238]

Substance	Phase	Year	Temperature Range of Heat Data, °K	Entropy at 298°K cal/°K-mol	Reference
tristearin: see 1,2,3-propanetriol, trioctadecanoate					
l-tryptophan. (l-α-amino-3-indolepropanoic acid), $C_8H_6NCH_2(NH_2)CHCOOH$	c	1963	tc, 12-301	60.00 (c)	[47]
	c	1964	tc, 0-300		
			th, 0-300	59.812 (c)	[13 R]
l-tyrosine: see l-2-amino-3(4-hydroxyphenyl)-propanoic acid					
undecanoic acid. (hendecanoic acid), $CH_3(CH_2)_9COOH$	c, l	1924	tc-, 273-339		[84]
undecolic acid: see undecanoic acid					
urea. (carbamide) $NH_2CONH_2$	soln	1899	tc-, 298 (100-400 moles H <sub>2</sub> O con- taining 1 mole urea)		[149]
	c	1920	tc, 86-300	41.0 ± 2 (c)	[89]
	c	1933	tc, 93-298	25.2 (c)	[185]
	soln	1935	tc, 289-312		
			(0.25-1.00 gm-mole/kg-H <sub>2</sub> O)		[77]
	soln	1936	tc, 293		
			(0.826-40% aq soln)		[26]
	soln	1936	tc, 298		
			(0.01-0.999 molar)		[258]
	soln	1937	tc, 275-313		
urea-ethanol mixture. $CH_4N_2O-C_2H_5OH$			(0-9.8 molarity)		[100]
	c	1946	tc, 19-318	25.00 ± 0.05 (c)	[207]
urea, 2-thio- . (thiocarbamide), $NH_2CSNH_2$			tc-, 298 (42.4-70.65 moles alcohol containing 1 mole urea)		[149]
	soln	1899			
urea, 2-thio- . (thiocarbamide), $NH_2CSNH_2$	c	1962	tc, 168-202		[257]
	g	1963	tc, 273.15-1000	72.44 (g)	[148]
uric acid: see 2,6,8-trihydroxypurine					
valeric acid: see pentanoic acid					
dl-valine: see dl-2-amino-3-methyl-butanoic acid					
l-valine: see d-2-amino-3-methyl-butanoic acid					
xanthine. (2,6-dioxypurine), $C_5H_4N_4O_2$	c	1935	tc, 85-298	38.5 (c)	[242]
zinc-insulin.	c	1964	tc, 10-305		[123]

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## Section II

### Heats and Free Energies of Formation of Compounds of C, H, N, O, P, and S

G. T. Armstrong and M. N. Inscoe

During the present reporting period, the work concerned with data on the heats and free energies of reaction was devoted to the assessment of available data and a continuing literature survey. Some of the results are summarized in the following tables.

A complete re-evaluation and selection of best values of heats of combustion and heats of formation was undertaken for eighteen organic compounds and the results of this study are given in Table 1. The compounds included in this study are compounds found in the Morowitz list of ubiquitous biochemical compounds, together with a few additional structurally-related compounds.

Calculations of free energies of formation at 298 °K were made for fourteen amino acids, using data given in previous progress reports. The results of these calculations are given in Table 2.

Table 3 is the supplementary list of compounds of C, H, N, O, P, and S containing not more than one carbon atom per molecule which was mentioned in NBS Report 8641, p. 8. While this list is quite inclusive, it cannot be regarded as complete. It is expected that a considerable number of inorganic compounds could be located in the section of Chemical Abstracts Collective Index 6 which was not available when the list was compiled. Some additional compounds might also be found in work published before the fifteen year period covered by the Chemical Abstracts Indexes consulted in making up the list, and still additional compounds could undoubtedly be found in the more recent literature. However, further attempts to obtain a complete list would seem to be of limited value. This list demonstrates the large number of compounds fitting into the present classification and suggests that the list of compounds could be extended indefinitely. The desirability of doing this is questionable.

In addition to the material given in these three tables, considerable work has been done on the literature files. The compound file mentioned in the previous report (NBS 8641, p. 8) which was set up for the ubiquitous biochemical compounds and structurally related compounds has been enlarged to include all compounds of C, H, N, O, P, and S listed in Table I, Section II of NBS Report 8595. At this time the file has not been expanded to include all known inorganic and one-carbon compounds

containing H, N, O, P, and S, but other compounds fitting this classification are being added to the file whenever thermodynamic data for them is encountered. The compounds in this file now number 560.

The bibliography file contains over 350 references; copies have been obtained of most of these sources. About a hundred additional references are on hand awaiting filing and classification with respect to compounds covered. All information referring to a particular compound is filed by compound in a compound reference file. Since most articles contain information on more than one compound, the compound reference file contains over two thousand items. Examination and evaluation of this material has not been completed. Many of the sources added to the files during the present reporting period have dealt with solution data and equilibrium data. The data on heats of solution and equilibria in solution may be of considerable importance in applications to prebiological systems.

Table 1  
Selected Heats of Combustion and Heats of Formation  
of Certain Organic Compounds

E. S. Domalski and I. Hallow

The data listed in this table are selected values obtained by complete reappraisal of the information in the references given. The heats of combustion and heats of formation in all cases are for the solid phase.

The selected heats of combustion and heats of formation for  $\beta$ -D-glucose and for  $\alpha$ -D-glucose hydrate were obtained by using heat of solution data for  $\alpha$ -D-glucose,  $\beta$ -D-glucose, and  $\alpha$ -D-glucose hydrate in conjunction with existing heat of combustion data on  $\alpha$ -D-glucose.

Compounds	$\Delta H_{c298}^{\circ}$ kcal mole <sup>-1</sup>	$\Delta H_{f298}^{\circ}$ kcal mole <sup>-1</sup>	References
Adenine	-664.25	+23.21	[26]
Creatine	-555.46	-128.16	[7,12,31]
Creatine hydrate	-552.8	-199.1	[31]
Creatine	-558.54	-56.77	[7,12]
Fumaric acid	-318.95	-193.89	[13,14,15,16,19,23,28,32,37]
$\alpha$ -D-Glucose	-669.94	-304.26	[5,7,9,13,20,21,22,24,25,27,29,30,33]
$\alpha$ -D-Glucose hydrate	-667.54	-374.97	[10,11,13,36]
$\beta$ -D-Glucose	-671.44	-302.76	[10,11,13,35,36]
Guanine	-597.33	-43.72	[26,31]
Hypoxanthine	-580.65	-26.24	[1,2,26]
Maleic acid	-323.89	-188.94	[13,14,15,16,19,23,30,37]
Nicotine	-1428.1	+9.4	[3,4]
8-Oxypurine	-591.4	-15.4	[1,2]
Pyruvic acid	-278.5	-140.3	[6]
D-Ribose*	-557.9	-253.9	[34]
Thymine	-563.3	-111.9	[8]
Uric acid	-459.16	-147.73	[7,17,18,26,27,29,31,33]
Xanthine	-516.39	-90.49	[3,4,26]

\* Crystalline D-ribose is in the  $\beta$ -pyranose form.  
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Table 2

## Free Energies of Formation of Certain Amino Acids

E. S. Domalski

The entropies and free energies of formation listed in this table were calculated from data given in previous reports. The heat of formation data were taken from Table 1, NBS Report 8641, p. 12. Entropy data were obtained from tables in NBS Report 8595, pp. 2-19 and 20-30.

Compound	$\Delta H_f^\circ_{298}$ kcal mole <sup>-1</sup>	$\Delta S_f^\circ_{298}$ cal deg <sup>-1</sup> mole <sup>-1</sup>	$\Delta G_f^\circ_{298}$ kcal mole <sup>-1</sup>
L-Alanine	-133.96	-154.34	-87.94
L-Asparagine hydrate	-259.52	-255.19	-183.44
L-Aspartic acid	-232.47	-194.94	-174.35
L-Cystine	-250.6	-287.39	-164.9
L-Glutamic acid	-240.05	-223.19	-173.51
L-Glutamine	-197.8	-235.53	-127.6
Glycine	-126.22	-127.88	-88.09
L-Isoleucine	-151.8	-233.33	-82.2
L-Leucine	-151.97	-232.37	-82.69
L-Phenylalanine	-111.9	-204.87	-50.8
L-Proline	-125.7	-179.97	-72.0
L-Tryptophan	-99.8	-237.29	-29.1
L-Tyrosine	-163.4	-229.28	-95.0
L-Valine	-148.2	-207.67	-86.3

### Table 3

#### Supplementary List of Compounds of CHNOPS Containing Not More Than One C Atom per Molecule

May N. Inscoe

This list gives compounds not found in Table I, Section II, of the Progress Report of 1 November 1964 (NBS Report 8595). The compounds are all those appropriate to the study that were found in the Formula Index of Chemical Abstracts Decennial Index 5 and the Formula Index covering carbon compounds from Chemical Abstracts Collective Index 6. The Formula Index covering the remaining elements was not yet available for Collective Index 6. The compounds are listed in order of their empirical formulas. Functional-group formulas and names are also given when available. While most of the compounds have been positively demonstrated, a few are speculative at this time.

Table 3

Supplementary List of Compounds of CHNOPS  
Containing Not More than One C Atom per Molecule

Empirical Formula	Functional-Group Formula	Name
CHNO	C=N-OH	Fulminic acid
CHNO <sub>2</sub> S	HOS(O)CN	Cyanosulfurous acid
CHNO <sub>3</sub> S	HOS(O <sub>2</sub> )CN	Cyanosulfuric acid
CHNS	HNCS	Isothiocyanic acid
CHN <sub>3</sub> S <sub>2</sub>	N <sub>3</sub> -C(=S)SH	Azidodithioformic acid
CHN <sub>3</sub> S <sub>2</sub>	S-N=N-NH-C=S	$\Delta^2$ -1,2,3,4-Thiatriazoline-5-thione
CHN <sub>5</sub>	N=N-N=N-N=CH	Pentazine
CHN <sub>5</sub> O <sub>2</sub>	N <sub>3</sub> C(=O)N <sub>2</sub> OH	Azidooxomethanediazonium hydroxide
CHO	C(OH)	Hydroxymethylidyne
CHO <sub>2</sub>	CO(OH)	Carboxy
CHO <sub>2</sub>	HC(=O)O	Formyloxy
CHP	HCP	Methinophosphide
CH <sub>2</sub> NO	H <sub>2</sub> NCO	Carbamoyl
CH <sub>2</sub> N <sub>2</sub>	HN=C=NH	Carbodiimide
CH <sub>2</sub> N <sub>2</sub>	HC=N=NH	Isodiazomethane
CH <sub>2</sub> N <sub>2</sub> O <sub>3</sub>	HC(NO <sub>2</sub> )=NOH	Nitrolic acid
CH <sub>2</sub> N <sub>2</sub> O <sub>6</sub>	CH <sub>2</sub> (ONO <sub>2</sub> ) <sub>2</sub>	Methylene nitrate
CH <sub>2</sub> N <sub>2</sub> O <sub>6</sub> S <sub>2</sub>	N <sub>2</sub> C(SO <sub>3</sub> H) <sub>2</sub>	Diazomethanedisulfonic acid
CH <sub>2</sub> N <sub>4</sub> O	H <sub>2</sub> N-C(=O)-N <sub>3</sub>	Carbamoyl azide
CH <sub>2</sub> N <sub>4</sub> O	N=N-NH-N(O)=CH	Tetrazole oxide
CH <sub>2</sub> N <sub>4</sub> O	HO-N=N-N=N=CH	1-Hydroxytetrazole
CH <sub>2</sub> N <sub>4</sub> O	HN-N=N-NH-C=O	2-Tetrazolin-5-one
CH <sub>2</sub> N <sub>4</sub> O	HN-N=N-N=COH	Tetrazol-5-ol
CH <sub>2</sub> N <sub>4</sub> S	S-N=N-N=C-NH <sub>2</sub>	5-Amino-1,2,3,4-thiatriazole
CH <sub>2</sub> N <sub>6</sub> O	HN=C(N <sub>3</sub> )N <sub>2</sub> OH	Azidoiminomethanediazonium hydroxide
CH <sub>2</sub> N <sub>6</sub> O	HN-N=N-N=C-N=N-OH	Tetrazole-5-diazo hydroxide
CH <sub>2</sub> N <sub>6</sub> O	HN-N=N-N=C-N <sub>2</sub> <sup>+</sup> OH <sup>-</sup>	Tetrazolediazonium hydroxide
CH <sub>2</sub> N <sub>6</sub> O <sub>2</sub>	O <sub>2</sub> NNHC(=NH)N <sub>3</sub>	1-Azido-N-nitroformamidine
CH <sub>2</sub> N <sub>6</sub> O <sub>2</sub>	HN-N=N-N=CNNHO <sub>2</sub>	5-Nitraminotetrazole
CH <sub>2</sub> OS <sub>2</sub>	H <sub>2</sub> COS <sub>2</sub>	Dithiocarbonic acid
CH <sub>2</sub> O <sub>2</sub> S	H <sub>2</sub> CO <sub>2</sub> S	Thiocarbonic acid
CH <sub>2</sub> O <sub>3</sub>	H(CO)OOH	Peroxyformic acid
CH <sub>2</sub> O <sub>4</sub>	HO(C=O)OOH	Peroxycarbonic acid
CH <sub>2</sub> S	HC(=S)H	Thioformaldehyde
CH <sub>2</sub> S <sub>2</sub>	HC(=S)SH	Dithioformic acid
CH <sub>3</sub> N	H <sub>2</sub> C=NH	Methylenimine
CH <sub>3</sub> NO	CH <sub>3</sub> NO	Nitrosomethane
CH <sub>3</sub> NOS	N <sub>2</sub> NC(=O)SH	Thiocarbamic acid
CH <sub>3</sub> NOS	H <sub>2</sub> NC(=SO)H	Thioformamide, S-oxide
CH <sub>3</sub> NOS	CH <sub>3</sub> NSO	N-sulfinylmethylamine (methylthionylamine)
CH <sub>3</sub> NOS	CH <sub>3</sub> SNO	Methyl thionitrite
CH <sub>3</sub> NOS <sub>7</sub>	SSSSSSS-N-CH <sub>2</sub> OH	



Table 3 (cont'd)

Empirical Formula	Functional-Group Formula	Name
$\text{CH}_3\text{NO}_2$	$\text{H}_2\text{NCOOH}$	Carbamic acid
$\text{CH}_3\text{NO}_2$	$\text{HC}(=\text{O})\text{NHOH}$	Formohydroxamic acid
$\text{CH}_3\text{NO}_3$	$\text{CH}_3\text{ONO}_2$	Methyl nitrate
$\text{CH}_3\text{NO}_5\text{S}$	$\text{HONC}\cdot\text{H}_2\text{SO}_4$	Compound of sulfuric acid and fulminic acid
$\text{CH}_3\text{NO}_5\text{S}$	$\text{O}_2\text{NCH}_2\text{SO}_3\text{H}$	Nitromethanesulfonic acid
$\text{CH}_3\text{NO}_5\text{S}$	$\text{ONOSO}_2\text{OCH}_3$	Methyl nitrosylsulfate
$\text{CH}_3\text{NS}$	$\text{HC}(=\text{S})\text{NH}_2$	Thioformamide
$\text{CH}_3\text{N}_3$	$\text{H}_2\text{N}-\text{NH}-\text{CN}$	Carbazonitrile
$\text{CH}_3\text{N}_3$	$\text{CH}_3\text{N}_3$	Azidomethane
$\text{CH}_3\text{N}_3\text{O}_2\text{S}$	$\text{H}_2\text{NC}(=\text{S})\text{NHNO}_2$	1-Nitro-2-thiourea
$\text{CH}_3\text{N}_3\text{O}_2\text{S}$	$\text{CH}_3\text{SO}_2\text{N}_3$	Methanesulfonyl azide
$\text{CH}_3\text{N}_3\text{O}_3$	$\text{O}_2\text{N}-\text{NH}-\text{CN}\cdot\text{H}_2\text{O}$	Nitrocyanamide, hydrate
$\text{CH}_3\text{N}_5$	$\text{H}_2\text{NC}(=\text{NH})\text{N}_3$	1-Azidoformamidine
$\text{CH}_3\text{N}_5$	$\text{HN}-\text{N}=\text{N}-\text{N}=\text{C}-\text{NH}_2$	5-Aminotetrazole
$\text{CH}_3\text{O}$	$\text{CH}_3-\text{O}$	Methoxy
$\text{CH}_3\text{O}$	$\text{HO}-\text{CH}_2$	Hydroxymethyl
$\text{CH}_3\text{OPS}$	$\text{CH}_3\text{P}(\text{O})\text{S}$	Methylthionophosphine oxide
$\text{CH}_3\text{O}_2$	$\text{CH}_3\text{O}_2$	Methyldioxy
$\text{CH}_3\text{O}_2\text{PS}$	$\text{CH}_3\text{OP}(\text{O})\text{S}$	O-Methyl phosphenothioate
$\text{CH}_3\text{O}_5\text{P}$	$\text{HCCOOP}_3\text{H}_2$	Formic acid, anhydride with $\text{H}_3\text{PO}_4$
$\text{CH}_3\text{PS}_3$	$\text{CH}_3\text{SPS}_2$	Methyl phosphenotrithioate
$\text{CH}_3\text{S}$	$\text{CH}_3\text{S}$	Methylthio
$\text{CH}_4\text{N}$	$\text{CH}_3\text{NH}$	Methylamidogen
$\text{CH}_4\text{NO}_5\text{P}$	$\text{N}_2\text{HCCOOP}_3\text{H}$	Carbamic acid, anhydride with $\text{H}_3\text{PO}_4$
$\text{CH}_4\text{N}_2$	$\text{HC}(=\text{NH})\text{NH}_2$	Formamidine
$\text{CH}_4\text{N}_2\text{O}$	$\text{NH}_4\text{NCO}$	Ammonium isocyanate
$\text{CH}_4\text{N}_2\text{O}$	$\text{HC}(=\text{NH})\text{NHOH}$	N-Hydroxyformamidine
$\text{CH}_4\text{N}_2\text{O}$	$\text{CH}_3\text{N}_2\text{OH}$	Methanediazonium hydroxide
$\text{CH}_4\text{N}_2\text{O}$	$\text{CH}_3\text{N}-\text{NO}$	N-Nitrosomethylamine
$\text{CH}_4\text{N}_2\text{O}_2$	$\text{H}_2\text{NNHCOOH}$	Carbazic acid
$\text{CH}_4\text{N}_2\text{O}_2$	$\text{H}_2\text{NOC}(=\text{O})\text{NH}_2$	O-Carbamoylhydroxylamine
$\text{CH}_4\text{N}_2\text{O}_2$	$\text{CH}_3\text{N}(\text{NO})\text{OH}$	N-Methyl-N-nitrosohydroxylamine
$\text{CH}_4\text{N}_2\text{O}_2$	$(\text{H}_3\text{NOH})(\text{CNO})$	Hydroxylamine cyanate
$\text{CH}_4\text{N}_2\text{O}_2$	$\text{CH}_3\text{NHNO}_2$	N-Nitromethylamine
$\text{CH}_4\text{N}_2\text{O}_2\text{S}$	$\text{H}_2\text{NC}(=\text{NH})\text{SO}_2\text{H}$	Aminoiminomethanesulfinic acid
$\text{CH}_4\text{N}_2\text{O}_3\text{S}_2$	$\text{CNSSO}_3\text{NH}_4$	Ammonium thiocyanatosulfonate
$\text{CH}_4\text{N}_2\text{O}_3\text{S}$	$\text{HOS}(=\text{O})\text{NHNHCOOH}$	3-Sulfino carbazic acid
$\text{CH}_4\text{N}_2\text{O}_4\text{S}$	$\text{H}_2\text{NC}(=\text{O})\text{NHSO}_3\text{H}$	Ureasulfonic acid
$\text{CH}_4\text{N}_2\text{S}$	$\text{NH}_4\text{CNS}$	Ammonium isothiocyanate
$\text{CH}_4\text{N}_2\text{S}$	$\text{HN}=\text{C}(\text{SH})\text{NH}_2$	2-Thiopseudourea
$\text{CH}_4\text{N}_2\text{S}$	$\text{H}_2\text{NNHCS}_2\text{H}$	Dithiocarbazic acid
$\text{CH}_4\text{N}_4\text{O}$	$\text{H}_2\text{NC}(=\text{NH})\text{NHNO}$	Nitrosoguanidine
$\text{CH}_4\text{N}_4\text{O}_2$	$\text{O}_2\text{NNHCN}\cdot\text{NH}_3$	Nitrocyanamide, $\text{NH}_3$ derivative
$\text{CH}_4\text{N}_4\text{O}_4$	$\text{CH}_2(\text{NHNO}_2)_2$	$\text{N}_2\text{N}'$ -Dinitromethanediamine

Table 3 (cont'd)

Empirical Formula	Functional-Group Formula	Name
$\text{CH}_4\text{N}_4\text{O}_6$	$\text{C}(\text{NO}_2)_3\text{NH}_4$	Nitroform, ammonium derivative
$\text{CH}_4\text{N}_6$	$\text{HN}-\text{N}=\text{N}-\text{N}=\text{C}-\text{NHNH}_2$	5-Hydrazinotetrazole
$\text{CH}_4\text{OP}_2$		Carbophosphide
$\text{CH}_4\text{OS}$	$\text{CH}_2(\text{SH})\text{OH}$	Mercaptomethanol
$\text{CH}_4\text{O}_2$	$\text{CH}_2(\text{OH})_2$	Methanediol
$\text{CH}_4\text{O}_2$	$\text{CH}_3\text{OOH}$	Methyl hydroperoxide
$\text{CH}_4\text{O}_2\text{S}$	$\text{CH}_3\text{SO}_2\text{H}$	Methanesulfinic acid
$\text{CH}_4\text{O}_2\text{S}_2$	$\text{CH}_3\text{S}(\text{O}_2)\text{SH}$	Methanesulfonic acid, thio-
$\text{CH}_4\text{O}_3$	$\text{HOCH}_2\text{OOH}$	Hydroxymethyl hydroperoxide
$\text{CH}_4\text{O}_3\text{S}$	$\text{HOCH}_2\text{SO}_2\text{H}$	Hydroxymethanesulfinic acid
$\text{CH}_4\text{O}_3\text{S}$	$\text{CH}_3\text{OSO}_2\text{H}$	Methyl sulfite
$\text{CH}_4\text{O}_3\text{S}_3$	$\text{CH}_3\text{OS}(\text{O}_2)\text{SSH}$	Methyl thioperoxy monosulfate
$\text{CH}_4\text{O}_4\text{S}$	$\text{HOCH}_2\text{SO}_3\text{H}$	Hydroxymethanesulfonic acid
$\text{CH}_4\text{O}_4\text{S}_2$	$\text{HOCH}(\text{SO}_3\text{H})_2$	Hydroxymethanedisulfonic acid
$\text{CH}_4\text{O}_4\text{S}_2$	$(\text{HO})_2\text{C}(\text{SO}_3\text{H})_2$	Dihydroxymethanedisulfonic acid
$\text{CH}_4\text{O}_9\text{S}_3$	$\text{CH}(\text{SO}_3\text{H})_3$	Methanetrissulfonic acid
$\text{CH}_4\text{P}_2\text{S}$		Thiocarbophosphide
$\text{CH}_4\text{S}_2$	$\text{H}_2\text{C}(\text{SH})_2$	Methanedithiol
$\text{CH}_4\text{S}_2$	$\text{CH}_3\text{SSH}$	Thiomethanesulfenic acid
$\text{CH}_4\text{S}_3$	$\text{CH}_3\text{SSSH}$	Methyl hydrotrisulfide
$\text{CH}_5\text{NO}$	$\text{H}_2\text{NCH}_2\text{OH}$	Aminomethanol
$\text{CH}_5\text{NO}_2\text{S}$	$\text{H}_2\text{NCH}_2\text{SO}_2\text{H}$	Aminomethanesulfinic acid
$\text{CH}_5\text{NO}_2\text{S}$	$\text{CH}_3\text{SO}_2\text{NH}_2$	Methanesulfonamide
$\text{CH}_5\text{NO}_3\text{S}$	$\text{H}_2\text{NCH}_2\text{OSO}_2\text{H}$	Aminomethanol, sulfite
$\text{CH}_5\text{NO}_3\text{S}$	$\text{H}_2\text{NCH}_2\text{SO}_3\text{H}$	Aminomethanesulfonic acid
$\text{CH}_5\text{NO}_3\text{S}$	$\text{H}_2\text{NSO}_3\text{CH}_3$	Methyl sulfamate
$\text{CH}_5\text{NO}_3\text{S}$	$\text{CH}_3\text{NHSO}_3\text{H}$	Methylsulfamic acid
$\text{CH}_5\text{NO}_6\text{S}_2$	$\text{CH}_3\text{N}(\text{SO}_2\text{OH})_2$	Methylimidodisulfuric acid
$\text{CH}_5\text{NO}_6\text{S}_2$	$\text{H}_2\text{NCH}(\text{SO}_2\text{OH})_2$	Aminomethanedisulfonic acid
$\text{CH}_5\text{N}_2\text{O}_3\text{P}$	$\text{H}_2\text{NCH}=\text{N}-\text{PO}(\text{OH})_2$	(Aminomethylene)phosphoramidic acid
$\text{CH}_5\text{N}_3\text{O}$	$\text{H}_2\text{NC}(\text{=NH})\text{NHOH}$	Hydroxyguanidine
$\text{CH}_5\text{N}_3\text{O}_3\text{S}$	$\text{H}_2\text{NC}(\text{=NH})\text{NHSO}_3\text{H}$	Amidinosulfamic acid
$\text{CH}_5\text{N}_3\text{O}_3\text{S}$	$\text{H}_2\text{N}-\text{SO}_2-\text{NH}-\text{CO}-\text{NH}_2$	Sulfamoylurea
$\text{CH}_5\text{N}_3\text{O}_3\text{S}$	$\text{H}_2\text{N}(\text{CS})\text{NH}_2 \cdot \text{HNO}_3$	Thiourea nitrate
$\text{CH}_5\text{N}_3\text{S}$	$\text{H}_2\text{NNHCS}-\text{NH}_2$	Thiosemicarbazide
$\text{CH}_5\text{N}_3\text{S}$	$\text{HCNS} \cdot \text{H}_2\text{NHNH}_2$	Thiocyanic acid, compound with hydrazine
$\text{CH}_5\text{N}_5\text{O}_2$	$\text{H}_2\text{NNHC}(\text{=NH})\text{NHNH}_2$	1-Amino-3-nitro-guanidine
$\text{CH}_5\text{OP}$	$\text{H}_2\text{POCH}_3$	Methyl phosphinite
$\text{CH}_5\text{O}_2\text{P}$	$\text{H}_2\text{P}(\text{O})\text{OCH}_3$	Methyl phosphinate
$\text{CH}_5\text{O}_3\text{P}$	$\text{CH}_3\text{OP}(\text{OH})_2$	Methyl phosphite
$\text{CH}_5\text{O}_3\text{P}$	$\text{H}_2\text{P}-\text{C}(\text{OH})_3$	Phosphinoorthoformic acid
$\text{CH}_5\text{O}_3\text{PS}$	$\text{CH}_3\text{OPO}_2\text{SH}_2$	Methyl phosphorothioate
$\text{CH}_5\text{O}_4\text{P}$	$\text{CH}_3\text{OP}(\text{=O})(\text{OH})_2$	Methyl phosphate
$\text{CH}_5\text{O}_4\text{P}$	$\text{HOCH}_2\text{P}(\text{=O})(\text{OH})_2$	(Hydroxymethyl)phosphonic acid
$\text{CH}_6\text{NO}_2\text{P}$	$(\text{H}_2\text{N})(\text{CH}_3)\text{P}(\text{=O})\text{OH}$	P-Methylphosphonamidic acid
$\text{CH}_5\text{O}_3\text{P}$	$\text{HOCH}_2\text{PH}(\text{O})\text{OH}$	(Hydroxymethyl)phosphinic acid

Table 3 (cont'd)

Empirical Formula	Functional-Group Formula	Name
$\text{CH}_6\text{NO}_3\text{P}$	$\text{CH}_3\text{NHP}(=\text{O})(\text{OH})_2$	(Aminomethyl)phosphonic acid
$\text{CH}_6\text{N}_2$	$\text{CH}_2(\text{NH}_2)_2$	Methanediamine
$\text{CH}_6\text{N}_2\text{O}_2\text{S}$	$\text{CH}_3\text{SO}_2\text{NHNH}_2$	Methanesulfonic acid, hydrazide
$\text{CH}_6\text{N}_2\text{O}_2\text{S}$	$\text{H}_2\text{NSO}_2\text{NHCH}_3$	Methylsulfamide
$\text{CH}_6\text{N}_2\text{O}_3$	$\text{H}_2\text{NCONH}_2 \cdot \text{H}_2\text{O}_2$	Urea, compound with $\text{H}_2\text{O}_2$
$\text{CH}_6\text{N}_2\text{O}_3\text{S}$	$\text{H}_2\text{NHNCH}_2\text{SO}_3\text{H}$	Hydrazinomethanesulfonic acid
$\text{CH}_6\text{N}_2\text{O}_4\text{S}_2$	$\text{CH}_2(\text{NHSO}_2\text{H})_2$	N,N'-Methylenebisamidosulfurous acid
$\text{CH}_6\text{N}_2\text{O}_4\text{S}_2$	$(\text{H}_2\text{N})_2\text{C}(\text{SO}_2\text{H})_2$	Diaminomethanedisulfinic acid
$\text{CH}_6\text{N}_2\text{O}_6\text{S}_2$	$\text{CH}_2(\text{NHSO}_3\text{H})_2$	Methanedisulfamic acid
$\text{CH}_6\text{N}_2\text{S}_2$	$\text{H}_2\text{NCS}_2\text{NH}_4$	Ammonium dithiocarbamate
$\text{CH}_6\text{N}_3\text{O}_3\text{P}$	$(\text{NH}_2)_2\text{C}=\text{NP}(=\text{O})(\text{OH})_2$	(Diaminomethylene)phosphoramidic acid
$\text{CH}_6\text{N}_3\text{O}_3\text{P}$	$\text{H}_2\text{NC}(=\text{NH})\text{NHP}(=\text{O})(\text{OH})_2$	Amidinophosphoramidic acid
$\text{CH}_6\text{N}_4\text{S}$	$(\text{H}_2\text{NNH})_2\text{C}=\text{S}$	Thiocarbohydrazide
$\text{CH}_6\text{N}_6$	$\text{H}_2\text{N}-\text{N}=\text{N}-\text{NH}-\text{C}(=\text{NH})\text{NH}_2$	2-Tetrazene-1-carboxamidine
$\text{CH}_6\text{O}_4$	$\text{HCOOH} \cdot 2\text{H}_2\text{O}$	Formic acid, hydrate
$\text{CH}_6\text{O}_6\text{P}_2$	$\text{CH}_2(\text{PO}_3\text{H}_2)_2$	Methylenediphosphonic acid
$\text{CH}_7\text{NO}_4\text{S}$	$\text{CH}_3\text{OSO}_3\text{NH}_4$	Ammonium methyl sulfate
$\text{CH}_7\text{N}_2\text{OP}$	$(\text{H}_2\text{N})_2\text{P}(=\text{O})\text{CH}_3$	P-Methylphosphonic diamide
$\text{CH}_7\text{N}_2\text{OP}$	$(\text{H}_2\text{N})_2\text{P}(\text{OCH}_3)$	Methyl phosphorodiamidite
$\text{CH}_7\text{N}_2\text{O}_2\text{P}$	$(\text{H}_2\text{N})_2\text{P}(=\text{O})\text{OCH}_3$	Methyl phosphorodiamidate
$\text{CH}_7\text{N}_2\text{O}_5\text{P}$	$\text{H}_3\text{PO}_4 \cdot \text{H}_2\text{NCONH}_2$	Phosphoric acid, compound with urea
$\text{CH}_7\text{N}_3$	$\text{HC}(\text{NH}_2)_3$	Methanetriamine
$\text{CH}_7\text{N}_3\text{O}$	$\text{H}_2\text{NC}(=\text{NH})\text{NH}_3\text{OH}$	Guanidinium hydroxide
$\text{CH}_7\text{N}_3\text{O}$	$\text{H}_2\text{NCONH}_2 \cdot \text{NH}_3$	Urea, compound with $\text{NH}_3$
$\text{CH}_7\text{N}_3\text{O}_2$	$\text{H}_2\text{NNH}_2 \cdot \text{CH}_3\text{NO}_3$	Hydrazine, compound with nitromethane
$\text{CH}_7\text{N}_3\text{O}_2$	$\text{CH}_3\text{N}=\text{N}(=\text{O})\text{ONH}_4$	N-aci-Nitromethylamine, ammonium derivative
$\text{CH}_7\text{N}_3\text{O}_4\text{S}_2$	$\text{CH}_3\text{N}(\text{SO}_2\text{NH}_2)_2$	N-Methylimidodisulfamide
$\text{CH}_7\text{N}_3\text{S}$	$\text{H}_2\text{NCSNH}_2 \cdot \text{NH}_3$	Thiourea, compound with $\text{NH}_3$
$\text{CH}_7\text{N}_5$	$\text{H}_2\text{NNHC}(=\text{NH})\text{NHNH}_2$	1,3-Diaminoguanidine
$\text{CH}_7\text{N}_5$	$\text{NHNHNHNHCH}-\text{NH}_2$	5-Aminotetrazolidine
$\text{CH}_7\text{N}_7$	$\text{HN}-\text{N}=\text{N}-\text{N}=\text{C}-\text{NH}_2 \cdot \text{H}_2\text{NNH}_2$	5-Aminotetrazole, compound with hydrazine
$\text{CH}_8\text{N}_2\text{O}$	$\text{H}_2\text{NNH}_2 \cdot \text{CH}_3\text{OH}$	Hydrazine, compound with methanol
$\text{CH}_8\text{N}_2\text{O}_3\text{S}$	$(\text{CH}_3\text{SO}_3)(\text{NH}_3\text{NH}_2)$	Methanesulfonic acid, hydrazine salt
$\text{CH}_8\text{N}_2\text{O}_5$	$\text{H}_2\text{NCONH}_2 \cdot 2\text{H}_2\text{O}_2$	Urea, compound with $\text{H}_2\text{O}_2$
$\text{CH}_8\text{N}_2\text{S}_3$	$(\text{NH}_4)_2\text{CS}_3$	Ammonium thiocarbonate
$\text{CH}_8\text{N}_4\text{O}_3\text{S}$	$\text{H}_2\text{NC}(=\text{NH})\text{NH}_3\text{SO}_3\text{NH}_2$	Guanidine, sulfamate
$\text{CH}_8\text{N}_4\text{O}_3\text{S}$	$\text{H}_2\text{NSO}_2\text{NHC}(=\text{O})\text{NH}_2 \cdot \text{NH}_3$	Sulfamoylurea, $\text{NH}_3$ derivative
$\text{CH}_8\text{N}_4\text{O}_4$	$\text{NH}_4\text{NO}_3 \cdot \text{H}_2\text{NCONH}_2$	Ammonium nitrate, compound with urea
$\text{CH}_8\text{N}_4\text{S}_2$	$\text{H}_2\text{NNHC}(=\text{S})\text{SH} \cdot \text{H}_2\text{NNH}_2$	Dithiocarbazic acid, hydrazine salt
$\text{CH}_8\text{N}_6$	$\text{H}_2\text{NNHC}(=\text{NNH}_2)\text{NHNH}_2$	Triaminoguanidine
$\text{CH}_8\text{N}_8$	$\text{H}_2\text{NNHC}(=\text{NH})\text{NHNH}_2 \cdot \text{HN}_3$	1,3-diaminoguanidine, hydrazoate
$\text{CH}_8\text{N}_8\text{O}_2$	$\text{HN}-\text{N}=\text{N}-\text{N}=\text{C}-\text{NHNO}_2 \cdot 2\text{NH}_3$	5-Nitraminotetrazole, diammonium derivative
$\text{CH}_9\text{N}_9$	$\text{H}_2\text{NNHC}(=\text{NNH}_2)\text{NHNH}_2 \cdot \text{HN}_3$	1,2,3-Triaminoguanidine, hydrazoate
$\text{CH}_{10}\text{N}_4\text{O}_3$	$(\text{H}_2\text{NNH}_3)_2\text{CO}_3$	Hydrazine, carbonate

Table 3 (cont'd)

Empirical Formula	Functional-Group Formula	Name
$\text{CH}_{10}\text{N}_{10}\text{O}_2$	$\text{HN}-\text{N}=\text{N}=\text{N}=\text{C}-\text{NHNO}_2 \cdot \text{H}_2\text{NNH}_2$	5-Nitraminotetrazole, compound with hydrazine
$\text{CH}_{11}\text{N}_2\text{O}_4\text{P}$	$\text{CH}_3\text{OPO}_3(\text{NH}_4)_2$	Ammonium methyl phosphate
$\text{CH}_{12}\text{N}_2\text{O}_9$	$\text{H}_2\text{NCONH}_2 \cdot 4\text{H}_2\text{O}_2$	Urea, compound with $\text{H}_2\text{O}_2$
CNO	CNO	Cyanato
CNO	NCO	Isocyanato
CNS	NCS	Isothiocyanato
$\text{CN}_2\text{OS}$	ONCNS	Nitrosyl thiocyanate
$\text{CN}_6$	$\text{N}=\text{N}-\text{N}=\text{N}-\text{C}=\text{N}=\text{N}$	5-Diazotetrazole
$\text{CO}_3$		Carbon oxide
CP		
$(\text{HN})_n$		Imidogen polymer
HNO	HNO	
HNOS	$\text{S}=\text{NOH}$	Sulfur oxide, oxime
HNOS	$\text{O}=\text{S}=\text{NH}$	Thionyl imide
$\text{HNO}_2\text{S}$	$\text{N}=\text{SO}_2\text{H}$	
$\text{HNO}_2\text{S}$	$\text{O}_2\text{S}=\text{NH}$	Sulfimide
$\text{HNO}_3$	$\text{ON}-\text{O}-\text{OH}$	Peroxynitrous acid
$\text{HNO}_3\text{S}_8$	$\text{SSSSSSS}-\text{N}-\text{SO}_3\text{H}$	Heptasulfuramidodisulfonic acid
$\text{HNO}_4$	$\text{O}_2\text{N}-\text{OOH}$	Peroxynitric acid
$\text{HNO}_6\text{S}$	$\text{O}_2\text{NOSO}_2\text{OH}$	Nitryl sulfate
$\text{HNO}_8\text{S}_2$	$\text{ONOSO}_2\text{OSO}_2\text{OH}$	Nitrosyl pyrosulfate
$\text{HNO}_9\text{S}_2$	$\text{HNO}_3 \cdot 2\text{SO}_3$	
$\text{HNO}_9\text{S}_2$	$\text{O}_2\text{NOSO}_2\text{OSO}_2\text{OH}$	Nitryl pyrosulfate
$\text{HNO}_{12}\text{S}_3$	$\text{HNO}_3 \cdot 3\text{SO}_3$	
$\text{HNO}_{12}\text{S}_3$	$\text{O}_2\text{NOSO}_2\text{OSO}_2\text{OSO}_2\text{OH}$	Nitryl trisulfate
$\text{HNO}_{15}\text{S}_4$	$\text{O}_2\text{NOSO}_2\text{OSO}_2\text{OSO}_2\text{OSO}_2\text{OH}$	Nitryl tetrasulfate
$\text{HNO}_{57}\text{S}_{18}$	$\text{HNO}_3 \cdot 18\text{SO}_3$	
HNS	$\text{S}=\text{NH}$	Sulfur imide
$\text{HNS}_7$	$\text{SSSSSSSNH}$	Heptasulfurimide
$\text{HN}_2\text{O}_6\text{S}$	$(\text{N}_2\text{O}_2)(\text{HSO}_4)$	
$\text{HN}_3\text{OS}_4$	$(\text{SN})_3\text{SOH}$	Tris(thionitroso)sulfonium hydroxide
HN	$\text{HN}-\text{N}=\text{N}=\text{N}$	Pentazole
$\text{HO}_3$	$\text{HO} \cdot \text{O}_2$	
$\text{HO}_4$	$\text{HO}_2 \cdot \text{O}_2$	
$\text{HPS}_3$	$\text{S}_2\text{PSH}$	Phosphenotritithioic acid
HS	HS	Mercapto
$\text{H}_2\text{NO}$	$\text{H}_2\text{NO}$	
$\text{H}_2\text{NS}_6$	$\text{S}_6\text{NH}_2$	
$\text{H}_2\text{N}_2$	$\text{H}-\text{N}=\text{N}-\text{H}$	Diimide
$\text{H}_2\text{N}_2\text{O}_2$	$\text{HON}=\text{NOH}$	Hyponitrous acid
$\text{H}_2\text{N}_2\text{O}_2$	$\text{O}_2\text{NNH}_2$	Nitramide
$\text{H}_2\text{N}_2\text{O}_5\text{S}$	$\text{ON}-\text{N}(\text{OH})\text{SO}_3\text{H}$	Nitrosyldihydroxylaminesulfonic acid
$\text{H}_2\text{N}_2\text{O}_6$	$[\text{NO}(\text{OH})_2]\text{NO}_3$	
$\text{H}_2\text{N}_2\text{O}_9\text{S}$	$2\text{HNO}_3 \cdot \text{SO}_3$	
$\text{H}_2\text{N}_2\text{O}_{15}\text{S}_3$	$2\text{HNO}_3 \cdot 3\text{SO}_3$	
$\text{H}_2\text{N}_2\text{O}_{18}\text{S}_4$	$4\text{SO}_3 \cdot \text{N}_2\text{O}_5 \cdot \text{H}_2\text{O}$	

Table 3 (cont'd)

Empirical Formula	Functional Group Formula	Name
$H_2N_2S$	$HN=S=NH$	Sulfur imide
$H_2N_4O_2S_6$	$[(SN)_2SOH]_2$	Tetrakis(thionitroso)dithionous acid
$H_2N_4O_{10}$	$2HNO_3 \cdot N_2O_4$	
$H_2OS$	$H_2SO$	Dihydrogen sulfoxide
$H_2O_2S$	$HO-S-OH$	Sulfoxylic acid
$H_2O_2S_2$	$HOS(=O)SH$	Thiosulfurous acid
$H_2O_3S_2$	$HOS(O_2)SH$	Thiosulfuric acid
$H_2O_4$		Hydrogen superoxide
$H_2O_5S_2$	$HOS(=O)OS(=O)OH$	Pyrosulfurous acid
$H_2O_6S_3$	$HOS(O_2)-S-SO_2OH$	Trithionic acid
$H_2O_6S_4$	$HOS(O_2)-SS-SO_2OH$	Tetrathionic acid
$H_2O_6S_5$	$HOS(O_2)-S_3-SO_2OH$	Pentathionic acid
$H_2O_6S_6$	$HOS(O_2)-S_4-SO_2OH$	Hexathionic acid
$H_2O_6S_7$	$HOS(O_2)-S_5-SO_2OH$	Heptathionic acid
$H_2O_6S_8$	$HOS(O_2)-S_6-SO_2OH$	Octathionic acid
$H_2O_6S_9$	$HOS(O_2)-S_7-SO_2OH$	Nonathionic acid
$H_2O_{10}S_3$	$HOS(O_2)OS(O_2)OSO_2OH$	Trisulfuric acid
$H_2O_{13}S_4$	$HOS(O_2)OS(O_2)OS(O_2)OSO_3H$	Tetrasulfuric acid
$H_2S_2$	$HSSH$	Hydrogen sulfide, hydrogen persulfide
$H_2S_3$	$HSSSH$	Hydrogen sulfide
$H_2S_4$	$HSSSSH$	Hydrogen sulfide
$H_2S_6$	$HSSSSSH$	Hydrogen sulfide
$H_3NO_2S$	$SO_2 \cdot NH_3$	
$H_3NO_2S$	$H_2NSO_2H$	Amidosulfurous acid
$H_3NO_4S$	$HONHSO_3H$	Hydroxylamine-N-sulfonic acid
$H_3NO_4S$	$H_2NOSO_3H$	Hydroxylamine-O-sulfonic acid
$H_3NO_4S_2$	$HN(SO_2H)_2$	Imidodisulfurous acid
$H_3NO_6S_2$	$HN(SO_3H)_2$	Imidodisulfuric acid
$H_3NO_7S$	$H_2SO_4 \cdot HNO_3$	
$H_3NO_7S$	$H_2NO_3HSO_4$	Nitric acidium (1+) sulfate
$H_3NO_7S_2$	$HON(SO_3H)_2$	Hydroxylamine disulfonic acid
$H_3NO_{10}S_2$	$H_2NO_3HS_2O_7$	Nitric acidium (1+) pyrosulfate
$H_3N_2$	$H_2NNH$	Hydrazyl
$(H_3N_2)_n$		Hydrazyl, polymer
$H_3N_2OP$	$HN=P(=O)NH_2$	Metaphosphimamide
$H_3N_3$	$HN=N-NH_2$	
$H_3N_3O_6S_3$	$SO_2-NH-SO_2-NH-SO_2-NH$	1,3,5,2,4,6-Trithiatriazine, 1,1,3,3,5,5-hexoxide
$H_3N_3O_9$	$N(OH)_3(NO_3)_2$	
$H_3N_3O_{12}S$	$3HNO_3 \cdot SO_3$	
$H_3N_3O_{21}S_4$	$3HNO_3 \cdot 4SO_3$	
$H_3N_3O_{24}S_5$	$3HNO_3 \cdot 5SO_3$	
$H_3O_2P$	$H_2P(=O)OH$	Phosphinic acid
$H_3O_2PS_2$	$OP(SH)_2OH$	Phosphorodithioic acid
$H_3O_3P$	$HP(=O)(OH)_2$	Phosphonic acid

Table 3 (cont'd)

Empirical Formula	Functional-Group Formula	Name
$H_3O_3PS$	$OP(OH)_2SH$	Phosphorothioic acid
$H_3O_5P$	$(HO)_2P(=O)OOH$	Peroxymonophosphoric acid
$H_3O_9P_3$	$H_3(PO_3)_3$	Metaphosphoric acid
$H_3PS_4$	$SP(SH)_3$	Phosphorotetrathioic acid
$H_4N$	$NH_4$	Ammonium
$H_4NO_3P$	$NH_4PO_3$	Ammonium metaphosphate
$H_4NO_3P$	$H_2NP(=O)(OH)_2$	Phosphoramidic acid
$H_4NO_8P_3$	$HOP(=O)OP(=O)(OH)OP(=O)(OH)NH$	Imidotrimetaphosphoric acid
$H_4N_2O_2S$	$H_2NNHS(=O)OH$	Hydrazinesulfinic acid
$H_4N_2O_2S$	$H_2NSO_2NH_2$	Sulfamide
$H_4N_2O_2S$	$NH_4N=SO_2$	Ammonium sulfimide
$H_4N_2O_2S_2$		
$H_4N_2O_3S$	$H_2NNHSO_3H$	Hydrazinesulfonic acid
$H_4N_2O_4S_3$	$H_2NSO_2-S-SO_2NH_2$	Trithionamide
$H_4N_2O_8S_3$	$HOSO_2NHSO_2NHSO_3H$	Diimidotrisulfuric acid
$H_4N_2O_{11}S_2$	$(SO_5NH)_2 \cdot H_2O$	
$H_4N_2O_{25}S_6$	$6SO_3 \cdot N_2O_5 \cdot 2H_2O$	
$H_4N_3O_5S$	$H_2SO_3N(=O)NO$	Dinitrososulfurous acid
$H_4N_4O_8S_4$	$SO_2NHSO_2NHSO_2NHSO_2NH$ <u>(2 2 2 2)</u>	1,3,5,7,2,4,6,8-Tetrathiatetrazocine, 1,1,3,3,5,5,7,7-octaoxide
$H_4N_4O_{27}S_5$	$5SO_3 \cdot 2N_2O_5 \cdot 2H_2O$	
$H_4N_4O_{27}S_5$	$4HNO_3 \cdot 5SO_3$	
$H_4N_4S_4$	<u>S-NH-S-NH-S-NH-S-NH</u>	1,3,5,7,2,4,6,8-Tetrathiatetrazocine
$H_4O_5P_2$	$HOPH(=O)P(=O)(OH)_2$	Diphosphorous acid
$H_4O_5P_2$	$HOPH(=O)OPH(=O)OH$	Pyrophosphorous acid
$H_4O_5S$	$H_2O_2 \cdot SO_3$	
$H_4O_5S$	$H_3OHSO_4$	Oxonium sulfate
$H_4O_6P_2$	$(HO)_2P(=O)P(=O)(OH)_2$	Hypophosphoric acid
$H_4O_6P_2$	$HOPH(=O)OP(=O)(OH)_2$	Ischypophosphoric acid
$H_4O_6P_2S_2$	$(HO)_2P(=S)-OO-P(=S)(OH)_2$	Thioperoxydiphosphoric acid
$H_4O_{12}P_4$	$H_4(P_4O_{12})$	Metaphosphoric acid
$H_4O_{35}S_{11}$	$2H_2SO_4 \cdot 9SO_3$	
$H_5NO_2$	$NH_3 \cdot H_2O_2$	Ammonia, compound with $H_2O_2$
$H_5NO_2$	$NH_4OOH$	Ammonium peroxide
$H_5NO_6P_2$	$HN(PO_3H_2)_2$	Imidodiphosphoric acid
$H_5NO_7S_2$	$NH_4HS_2O_7$	Ammonium pyrosulfate
$H_5NO_{11}S_2$	$H_3NO_3(HSO_4)_2$	Nitric acidium(2+) sulfate
$H_5N_2O_2P$	$(H_2N)_2P(=O)OH$	Phosphorodiamidic acid
$H_5N_2O_7P_3$	$HOP(=O)OP(=O)(OH)NHP(=O)(OH)-NH$	Diimidotrimetaphosphoric acid
$H_5N_3O_2S_2$	$HN(SONH_2)_2$	Imidodisulfurous diamide
$H_5N_3O_4S_2$	$HN(SO_2NH_2)_2$	Imidodisulfamide
$H_5N_5O_{10}S_5$	<u><math>SO_2NHSO_2NHSO_2NHSO_2NH</math></u> <u>(2 2 2 2 2)</u>	1,3,5,7,9,2,4,6,8,10-Pentathiapentazecine, 1,1,3,3,5,5,7,7,9,9-decaoxide
$H_5O_{10}P_3$	$(HO)_2P(=O)OP(=O)(OH)OP(=O)(OH)_2$	Triphosphoric acid
$H_6NO_9P_3$	$(HO)_2P(=O)OP(=O)(OH)NHP(=O)(OH)_2$	Imidotriphosphoric acid
$H_6N_2$	$NH_4NH_2$	Ammonium amide
$H_5NO$	$NH_3 \cdot H_2O$	

Table 3 (cont'd)

Empirical Formula	Functional-Group Formula	Name
$H_6N_2O_2$	$N_2H_5OOH$	
$H_6N_2O_2S$	$H_2NSO_2NH_4$	Ammonium amidosulfite
$H_6N_2O_2S_2$	$H_2NS_2O_3NH_4$	Ammonium amidodithiosulfate
$H_6N_2O_3S$	$HONHSO_3NH_4$	Ammonium hydroxylaminesulfonate
$H_6N_2O_5S_3$	$H_2NSO_2SSO_3NH_4$	Ammonium amidotetrithionate
$H_6N_2O_{20}S_4$	$4SO_3 \cdot N_2O_5 \cdot 3H_2O$	
$H_6N_3OP$	$(H_2N)_3PO$	Phosphoric triamide
$H_6N_3O_5P_3$	$[PO(OH)NH]_3$	Metaphosphimic acid, trimer
$H_6N_3PS$	$(H_2N)_3PS$	Phosphorothioic triamide
$H_6N_4$	$H_2NNHNNH_2$	Tetrazane
$H_6N_4O_6$	$H_3NNH_3(NO_3)_2$	Hydrazine dinitrate
$H_6N_4O_9$	$NH_4NO_3 \cdot 2HNO_3$	Ammonium nitrate
$H_6O_4$	$H_2O_2 \cdot 2H_2O$	
$H_6O_6S$	$(HO)_6S$	Orthosulfuric acid
$H_6O_{12}S_2$	$2HOSO_2OOH \cdot H_2O_2$	Peroxymonosulfuric acid, compound with $H_2O_2$
$H_6O_{13}P_4$	$HO[-P(=O)(OH)O-]_4H$	Tetraphosphoric acid
$H_6O_{18}P_6$	$(HPO_3)_6$	Metaphosphoric acid
$H_7NO_6P_2$	$NH_4HP_2O_6$	Ammonium hypophosphate
$H_7N_2O_3P$	$H_2NPO_3HNH_4$	Ammonium phosphoramidate
$H_7N_5O_{14}S_6$	$HOSO_2^-(NHSO_2^-)_5OH$	Pentaimidohexasulfuric acid
$H_7O_6P$	$H_7(PO_6)$	
$H_8N_2O$	$2NH_3 \cdot H_2O$	
$H_8N_2O$	$(NH_4)_2O$	Ammonium oxide
$H_8N_2O_4S_2$	$(NH_4)_2S_2O_4$	Ammonium dithionite
$H_8N_2O_5S$	$(NH_4)_2SO_5$	Ammonium peroxymonosulfate
$H_8N_2O_6P_2$	$(NH_4)_2P_2O_6$	Ammonium metaphosphate
$H_8N_2O_6S_3$	$(NH_4)_2(O_3S-S-SO_3)$	Ammonium trithionate
$H_8N_2O_6S_4$	$(NH_4)_2(O_3S-SS-SO_3)$	Ammonium tetrathionate
$H_8N_2O_{10}S_3$	$(NH_4)_2(O_3SOSO_2OSO_3)$	Ammonium trisulfate
$H_8N_2O_{18}S_2$	$(SO_4NO_3)_2 \cdot 4H_2O$	
$H_8N_2O_{18}S_2$	$NO(OH)_4 \cdot S_2O_8 \cdot NO(OH)_4$	Nitropersulfuric acid
$H_8N_2O_{24}S_5$	$5SO_3 \cdot N_2O_5 \cdot 4H_2O$	
$H_8N_3O_2P$	$NH_4PO_2(NH_2)_2$	Ammonium phosphorodiamidate
$H_8N_4O_4S_2$	$HN(SO_2NH_2)_2 \cdot NH_3$	Imidodisulfamide, ammonium derivative
$H_8N_4O_5S$	$(NH_4)_2ONN(O)SO_3$	Ammonium nitrosohydroxylaminesulfonate
$H_7NO_8P_2$	$NH_4H_2PO_4 \cdot H_3PO_4$	Ammonium phosphate
$H_9N_2O_3PS$	$P(S)O_3H(NH_4)_2$	Ammonium phosphorothioate
$H_9N_3O_4S_2$	$HN(SO_2NH_4)_2$	Ammonium imidodisulfite
$H_9N_3O_6S_2$	$HN(SO_3NH_4)_2$	Ammonium imidodisulfate
$H_9N_3O_7S_2$	$HON(SO_3NH_4)_2$	Ammonium hydroxylamine disulfonate
$H_{10}N_2O_6S$	$(NH_4)_2SO_4 \cdot H_2O_2$	Ammonium sulfate, compound with $H_2O_2$
$H_{10}N_2O_7P_2$	$(NH_4)_2H_2P_2O_7$	Ammonium pyrophosphate
$H_{10}N_4O_2S$	$SO_2(NH_2)_2 \cdot 2NH_3$	
$H_{10}N_4O_5S_2$	$H_2NSO_2OSO_2NH_2 \cdot 2NH_3$	Pyrosulfamide, ammonium derivative
$H_{10}O_{26}S_7$	$5H_2SO_4 \cdot 2SO_3$	

Table 3 (cont'd)

Empirical Formula	Functional-Group Formula	Name
$H_{11}N_3O_7S_2$	$(NH_4)_2SO_4 \cdot HSO_3NH_2$	Hydroxylamine, phosphate
$H_{12}N_3O_7P$	$(HONH_3)_3PO_4$	Ammonium metaphosphate
$H_{12}N_3O_9P_3$	$(NH_4)_3(PO_3)_3$	Ammonium imidodisulfate
$H_{12}N_4O_6S_2$	$NH_4N(SO_3NH_4)_2$	Ammonium nitridotrisulfate
$H_{12}N_4O_9S_3$	$N(SO_3NH_4)_3$	Metaphosphimic acid, tetramer, dihydrate
$H_{12}N_4O_{10}P_4$	$[PO(OH)NH]_4 \cdot 2H_2O$	1,3,5,2,4,6-Trithiatriazine hexaoxide, N- ammonium derivative
$H_{12}N_6O_6S_3$	$SO_2-N-SO_2-N-SO_2-N(NH_4)_3$	Ammonium sulfate
$H_{13}N_3O_8S_2$	$(NH_4)_3H(SO_4)_2$	
$H_{13}N_5O_2S$	$SO_2(NH_2)_2 \cdot 3NH_3$	Ammonium metaphosphimate
$H_{14}N_6O_8P_4$	$[PO(OH)NH]_4 \cdot 2NH_3$	Ammonium phosphate
$H_{15}N_3O_8P_2$	$(NH_4)_3PO_4 \cdot H_3PO_4$	
$H_{15}N_5O_6S_2$	$(NH_4SO_3)_2NNH_4 \cdot NH_3$	
$H_{16}N_4O_7P_2$	$(NH_4)_4P_2O_7$	Ammonium pyrophosphate
$H_{16}N_6O_{10}S$	$2NH_4NO_3 \cdot (NH_4)_2SO_4$	Ammonium nitrate sulfate
$H_{17}N_5O_4S$	$(NH_4)_2SO_4 \cdot 3NH_3$	
$H_{18}N_2O_{44}S_{10}$	$10SO_3 \cdot N_2O_5 \cdot 9H_2O$	
$H_{18}N_4O_{52}S_{11}$	$11SO_3 \cdot 2N_2O_5 \cdot 9H_2O$	
$H_{19}NO_3S_9$	$9H_2SO_4 \cdot HNO_3$	
$H_{20}N_2O_{42}S_9$	$9H_2SO_4 \cdot 2HNO_3$	
$H_{21}N_3O_{16}P_4$	$(NH_4)_3PO_4 \cdot 3H_3PO_4$	Ammonium phosphate
$H_{24}N_9O_{13}P$	$3NH_4NO_3 \cdot (NH_4)_3PO_4$	Ammonium nitrate phosphate
$H_{26}N_6O_{16}S_4$	$H_2(NH_4)_6(SO_4)_4$	Ammonium sulfate
$H_{28}N_{22}O_{78}S_3$	$3H_2SO_4 \cdot 22HNO_3$	
$H_{30}N_7O_{12}P_3$	$H_2(NH_4)_7(PO_4)_3$	Ammonium phosphate
$NO_4$		Nitrogen oxide
$(NS)_n$	$(SN)_n$	Sulfur nitride
$N_2OS_3$	$(NS)_2SO$	
$N_2O_2$	$ONNO$	Nitrogen oxide
$N_2O_2S_3$	$SOS(=O)N=S=N$	Trisulfur dinitrogen dioxide
$N_2O_5S_3$	$SO_2N=S=NSO_2$	Trisulfur dinitrogen pentoxide
$N_2O_5S_4$	$O_3S-N-S=N-S(=O)-O-S$	
$N_2O_9S_2$	$(NO)_2S_2O_7$	Nitrosyl pyrosulfate
$N_2O_{11}S_2$	$(NO_2)_2S_2O_7$	Nitryl pyrosulfate
$N_2O_{12}S_3$	$(NO_2)_2S_3O_{10}$	Nitrosyl trisulfate
$N_2O_{13}S_3$	$(NO)(NO_2)S_3O_{10}$	Nitrosyl nitryl trisulfate
$N_2O_{14}S_3$	$N_2O_5 \cdot 3SO_3$	
$N_2O_{14}S_3$	$(NO_2)_2S_3O_{10}$	Nitryl trisulfate
$N_2O_{17}S_4$	$N_2O_5 \cdot 4SO_3$	
$N_2O_{17}S_4$	$(NO_2)_2S_4O_{13}$	Nitryl tetrasulfate
$N_2S_2$	$S_2N_2$	Sulfur nitride
$N_2S_4$	$SNSSNS$	Sulfur nitride
$N_2S_5$	$S_5N_2$	Sulfur nitride
$N_3O_{10}P$	$PO(NO_3)_3$	Phosphoryl nitrate
$N_4O$	$(NO)_N_3$	Nitrosyl azide
$N_4O_6S_6$	$N_4S_4 \cdot 2SO_3$	Sulfur nitride, compound with $SO_3$
$H_{16}N_4O_{12}P_4$	$(NH_4)_4(PO_3)_4$	Ammonium metaphosphate



Table 3 (cont'd)

Empirical Formula	Functional-Group Formula	Name
$N_4O_{12}S_8$	$N_4S_4 \cdot 4SO_3$	Sulfur nitride, compound with $SO_3$
$N_4O_4S_{11}$	$2N_2O_5 \cdot 11SO_3$	
$N_4S_4$	$S_4N_4$	Sulfur nitride
$N_5P_3$	$P_3N_5$	Phosphorus nitride
$N_{21}P_3$	$[NP(N_3)_2]_3$	Phosphonitrile azide, trimer
$OS_2$	$S_2O$	Disulfur monoxide
$O_2S_2$	$S_2O_2$	Sulfur oxide
$O_3S_2$	$S_2O_3$	Disulfur trioxide
$O_4$	$O_4$	Oxygen, tetratomic
$O_4S$	$SO_4$	Sulfur tetroxide
$O_6P_4S_4$	$P_4S_4O_6$	Phosphorus oxysulfide
$O_7S_2$	$S_2O_7$	Disulfur heptoxide
$O_{10}P_6S_5$	$P_6S_5O_{10}$	Phosphorus oxysulfide
$O_{14}P_2S_3$	$P_2O_5 \cdot 3SO_3$	
$P_2S_5$	$P_2S_5$	Phosphorus sulfide
$P_3S_6$	$P_3S_6$	Phosphorus sulfide
$P_4S_5$	$P_4S_5$	Phosphorus sulfide
$P_4S_6$	$P_4S_6$	Phosphorus sulfide
$P_4S_7$	$P_4S_7$	Phosphorus sulfide
$P_4S_{10}$	$P_4S_{10}$	Phosphorus sulfide

# SUMMARY INDEX

TABLES IN NBS REPORTS 8521, 8595, 8641, AND 8906

Report Number	Title of Table	Page No.
8521	Section I.	
	Preliminary compilation of heat capacity and relative enthalpy and entropy data published on biologically related substances . . .	5
	Section II.	
	Preliminary compilation of data on heats and free energies of reaction and formation: bibliography on amino acids . . . . .	33
	Preliminary list of compounds of C, H, N, O, P, and S containing not more than one carbon atom per molecule . . . . .	49
8595	Section I.	
	Analysis of heat-capacity data on some amino-acids	
	Table 1. Molal thermodynamic functions for glycine . . . . .	3
	Table 2. Molal thermodynamic functions for L-alanine . . . . .	4
	Table 3. Molal thermodynamic functions for L-valine . . . . .	5
	Table 4. Molal thermodynamic functions for L-leucine . . . . .	6
	Table 5. Molal thermodynamic functions for L-isoleucine . . . . .	7
	Table 6. Molal thermodynamic functions for L-tyrosine . . . . .	8
	Table 7. Molal thermodynamic functions for L-phenylalanine . . . . .	9
	Table 8. Molal thermodynamic functions for L-tryptophane . . . . .	10
	Table 9. Molal thermodynamic functions for L-aspartic acid . . . . .	11
	Table 10. Molal thermodynamic functions for L-asparagine monohydrate . .	12
	Table 11. Molal thermodynamic functions for L-glutamic acid . . . . .	13
	Table 12. Molal thermodynamic functions for L-glutamine . . . . .	14
	Table 13. Molal thermodynamic functions for L-lysine hydrochloride . .	15
	Table 14. Molal thermodynamic functions for L-arginine hydrochloride . .	16
	Table 15. Molal thermodynamic functions for L-histidine hydrochloride .	17
	Table 16. Molal thermodynamic functions for L-cystine . . . . .	18
	Table 17. Molal thermodynamic functions for L-proline . . . . .	19
	Section II.	
	Table 1. Preliminary table of selected thermodynamic data on compounds of C, H, N, O, P, and S containing not more than one carbon atom per molecule . . . . .	21
8641	Section I.	
	Partial survey of heat-capacity data on "ubiquitous biochemical compounds"	
	Table I. "Ubiquitous substances" on which no heat-capacity data have been found . . . . .	2
	Table II. "Ubiquitous substances" on which heat-capacity data exist and which have previously been surveyed . . . . .	4
	Table III. "Ubiquitous substances" on which heat-capacity data exist . .	6
	Section II.	
	Table 1. Selected heats of combustion and heats of formation of amino acids and some polypeptides . . . . .	12
	Table 2. Partial list of thermodynamic data on ubiquitous biochemical compounds and some related compounds . . . . .	14
	Table 3. Ubiquitous compounds — Formula index . . . . .	28
8906	Section I.	
	References to Heat Capacity, Enthalpy, and Entropy Data on CHNOPS Compounds . . . . .	5
	Section II.	
	Table 1. Selected heats of combustion and heats of formation of certain organic compounds . . . . .	71
	Table 2. Free energies of formation of certain amino acids . . . . .	74
	Table 3. Supplementary list of compounds of C, H, N, O, P, and S containing not more than one carbon atom per molecule . . . . .	76

\* For two corrections to this table, see the introduction to the present report.